temperature, shows a rapid loss of spectral weight below about 40 meV for far-infrared reflectance continues to increase; however, the reflectance over much of the infrared is suppressed. The conductivity, Drude-like above the ordering to the estimate of the gap maximum to the pseudogap in the normal state of the cuprates. Instead, the gapping of the normal-state single-particle excitations looks surprisingly similar to that observed in $T \sim 25$ meV) signaling the formation of a superconducting energy gap; the suppression of the conductivity for the reflectance increases monotonically over the far-infrared frequency range, with an abrupt increase in the reflectance below a wide frequency and temperature range. The optical conductivity has been determined from a Kramers-Kronig analysis. In the slightly underdoped material, superconductors 1, 2 and J. C. Davis. This work done in collaboration with S.V. Dordevic, G.D. Gu, Q. Li, T. Valla, and J.M. Tranquada. Supported by the U.S. Department of Energy, under Contract No. DE-AC02-98CH10886.

8:36AM A1.00002 An intrinsic Cu-O-Cu bond-centered electronic glass with disperse 4 $a_0$-wide unidirectional domains in strongly underdoped Ca$_{1.88}$Na$_{0.12}$Cu$_2$O$_2$Cl$_2$ and Bi$_2$Sr$_2$DY$_{0.2}$Ca$_{0.8}$Cu$_2$O$_y$. YUHKI KOHSAKA, Cornell University — Hole doping into the CuO$_2$ charge transfer insulator alters the electronic correlations, leading to the high-$T_c$ superconductivity (HTS). The correlation alterations are accompanied by spectral weight transfers from the high energy states of the insulator to low energies. Recently, it has been proposed [1,2] that these effects might be observable as an asymmetry of electron tunneling currents with bias voltage across the chemical potential. Atomic-scale TA-phenomena would then be of crucial importance to understand the fundamental electronic structure of the CuO$_2$ plane from whence the HTS emerges.

In this talk, we will report on the topological atomic resolution TA-imaging by STM, detecting virtually identical phenomena in two different lightly hole-doped cuprates: Ca$_{1.88}$Na$_{0.12}$Cu$_2$O$_2$Cl$_2$ and Bi$_2$Sr$_2$DY$_{0.2}$Ca$_{0.8}$Cu$_2$O$_y$. We find intense spatial variation primarily on planer oxygen sites. Their spatial arrangements appear to be a Cu-O-Cu bond-centered electronic glass, breaking translational symmetry of lattice and $90^\circ$-rotational symmetry. 4 $a_0$-wide unidirectional domains (4 $a_0$: Cu-O-Cu length) are embedded throughout this matrix and running along the both Cu-O bonds without preferred orientation. Relationship to the electronic cluster glass, the bond-centered stripe, and the high-$T_c$ superconductivity will be discussed. This work is done in collaboration with C. Taylor, A. Schmidt, C. Lupien, T. Hanaguri, M. Azuma, M. Takano, K. Fujita, H. Eisaki, H. Takagi, S. Uchida, and J. C. Davis.


9:12AM A1.00003 Nature of the electronic gap in stripe-ordered cuprates 1, CHRISTOPHER HOMES, Brookhaven National Laboratory — The ab-plane optical properties of single crystals of the high-temperature superconductor La$_{2-x}$Ba$_x$CuO$_4$, with chemical dopings of $x = 0.005$ (slightly underdoped) and 0.125 (1/8 doping) and critical temperatures ($T_c$'s) of 32 and $\gtrsim 2.4$ K, respectively, have been measured over a wide frequency and temperature range. The optical conductivity has been determined from a Kramers-Kronig analysis. In the slightly underdoped material, the reflectance increases monotonically over the far-infrared frequency range, with an abrupt increase in the reflectance below $T_c$ below about 200 cm$^{-1}$ (about 25 meV) signaling the formation of a superconducting energy gap: the suppression of the conductivity for $T < T_c$ occurs below this energy. This is close to the estimate of the gap maximum 2$\Delta_0$ determined from angle resolved photoemission spectroscopy. In contrast, the 1/8 doping shows a dramatically different behavior $[T$ the reflectance increases monotonically with decreasing temperature. Below $\sim 60$ K, corresponding to the onset of charge-stripe order, the far-infrared reflectance continues to increase; however, the reflectance over much of the infrared is suppressed. The conductivity, Drude-like above the ordering temperature, shows a rapid loss of spectral weight below about 40 meV for $T < 60$ K. This behavior is quite different from that typically associated with the pseudogap in the normal state of the cuprates. Instead, the gapping of the normal-state single-particle excitations looks surprisingly similar to that observed in superconducting La$_{2-x}$Sr$_x$CuO$_4$, including the presence of a residual Drude peak with reduced weight.

1This work done in collaboration with S.V. Dordevic, G.D. Gu, Q. Li, T. Valla, and J.M. Tranquada. Supported by the U.S. Department of Energy, Division of Materials Science, under Contract No. DE-AC02-98CH10886.

9:48AM A1.00004 Neutron scattering evidence for spin and charge inhomogeneity in cuprate superconductors 1, JOHN TRANQUADA, Brookhaven National Lab — Neutron diffraction studies have provided clear evidence for charge and spin stripe order in La$_{2-x}$Ba$_x$CuO$_4$ and La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ for a range of $x$, with a maximum ordering temperature at $x = 1/8$. The ordering of stripes competes with superconducting order. Recent measurements of the magnetic excitation spectrum in La$_{2.375}$Ba$_{1.625}$CuO$_4$ show that: 1) the energy scale corresponds to antiferromagnetic superexchange, 2) the qualitative features do not change when static stripe order disappears $[1]$, and 3) the spectrum is very similar to that found in other cuprate superconductors. New measurements on optimally-doped Bi$_2$Sr$_2$Ca$_2$Cu$_2$O$_{8+\delta}$ $[2]$ are consistent with the concept of a universal spectrum. Results on over-doped La$_{2-x}$Sr$_x$CuO$_4$ show that the magnetic spectral weight disappears as the superconductivity goes away $[3]$. These results suggest that slowly-fluctuating charge inhomogeneity is common to the cuprates and underlies the high-temperature superconductivity.

1This work is supported by the Office of Science, U.S. Department of Energy, under Contract No. DE-AC02-98CH10886.
10:24AM A1.00005 Duality and the vibrational modes of a Cooper-pair Wigner crystal. MARCEL FRANZ, University of British Columbia — When quantum fluctuations in the phase of the superconducting order parameter destroy the off-diagonal long range order, duality arguments predict the formation of a Cooper pair Wigner crystal. This effect is thought to be responsible for the static checkerboard patterns observed recently in various underdoped cuprate superconductors by means of scanning tunneling spectroscopy. I will sketch the calculation of the vibrational modes of this pair crystal using a continuum version of the standard vortex-boson duality. Such calculations yield bounds on the sound velocity of the phonon modes which are in agreement with the numbers extracted from the thermal conductivity measurements but indicate that vibrations are robustly three dimensional in nature. Generalization of the inherently two-dimensional vortex-boson duality to three dimensions is outlined and an intriguing connection to the theory of bosonic strings is pointed out.

Monday, March 5, 2007 8:00AM - 11:00AM –
Session A3 DCMP: Electronic States in Graphene Colorado Convention Center Korbel 2A-3A

8:00AM A3.00001 Infrared Probe of the Anomalous Magneto-transport of Graphite in the Extreme Quantum Limit. DMITRI BASOV, UCSD — We present a systematic investigation of the magnetoreflectance of highly oriented pyrolytic graphite in magnetic fields B up to 18 T. From these measurements, we report the determination of lifetimes tau associated with the lowest Landau levels in the quantum limit. We find a linear field dependence for inverse lifetime 1/tau(B) of the lowest Landau levels, which is consistent with the hypothesis of a three-dimensional (3D) to 1D crossover in an anisotropic 3D metal in the quantum limit. This enigmatic result uncovers the origin of the anomalous linear in-plane magnetoresistance observed both in bulk graphite and recently in mesoscopic graphite samples. This work is a collaboration with Z.Q. Li, S.-W. Tsai, W.J. Padilla, S.V. Dordevic, K.S. Burch, and Y.J. Wang.

8:36AM A3.00002 Two-Dimensional Dirac Fermions in Graphene at High Magnetic Fields. YUANBO ZHANG, Department of Physics, University of California at Berkeley — Graphene, a single atomic sheet of graphite, is a monolayer of carbon atoms densely packed into a honeycomb structure. It can be viewed as either an unrolled single-wall carbon nanotube or a giant flat fullerene molecule. Advances in micromechanical extraction and fabrication techniques for graphene structures now permit such exotic 2D electron systems to be probed experimentally. It has been discovered that the electrons in graphene are two-dimensional Dirac Fermions, based on the observation of half-integer quantum Hall effect and Berry’s phase of ω in the magneto-oscillations. We further investigate the transport properties of graphene in extremely strong magnetic fields. Under such condition, we observe new sets of quantum Hall states at filling factors ν = 0, ±1, ±4, indicating the lifting of the four-fold degeneracy of the previously observed quantum Hall states at ν = ±4(n+1/2), where n is the Landau level index. In particular, the presence of the ν = 0, ±1 quantum Hall states indicates that the Landau level at the charge neutral Dirac point splits into four sub-levels, lifting both sublattice and spin degeneracy in graphene. The quantum Hall effect at ν = ±1, ±4 is studied in tilted magnetic fields at various temperatures. It has been found that ν = ±4 are due to the lifting of the spin-degeneracy of the Landau level n = ±1 while ν = ±1 are most likely due to the sublattice degeneracy lifting of n = 0. Finally, the availability of large, high quality graphene crystals opens new possibilities for optical and scanning probe studies. A brief discussion of our recent experiments on Raman spectroscopy and STM will be presented.

9:12AM A3.00003 Electronic Confinement and Coherence in Patterned Epitaxial Graphene. CLAIRE BERGER, GATECH-Atlanta / CNRS-France — Transport in ultrathin graphite films grown on single-crystal silicon carbide is dominated by the electron-doped epitaxial graphene layer at the interface and shows graphene characteristics. Epitaxial graphene provides a platform for studying the novel electronic properties of this 2D electron gas in a controlled environment. Shubnikov-de Haas oscillations in the magnetoresistance data indicate an anomalous Berry’s phase and reveal the Dirac nature of the charge carriers. The system is highly coherent with phase coherence lengths beyond 1 micrometer at cryogenic temperatures, and mobilities exceeding 2.5 square meters per volt-second. In wide structures, evidence is found for weak anti-localization in agreement with recent graphene weak-localization theory. Patterned narrow ribbons show quantum confinement of electrons. Several Hall bar samples reveal anomalous magnetoresistance patterns consisting of large structured non-periodic oscillations that may be due to a periodic superlattice potential.


10:24AM A3.00005 Electronic properties of single and multi-layer Graphene. ANTONIO CASTRO NETO, Boston University — Graphene, a two dimensional carbon crystal with a honeycomb lattice, was discovered only two years ago. It has generated a lot of new possibilities for optical and scanning probe studies. A brief discussion of our recent experiments on Raman spectroscopy and STM will be presented.

Monday, March 5, 2007 8:00AM - 11:00AM –
Session A7 DCMP: Unconventional Transport and Magnetic Properties of Hexaborides Colorado Convention Center Korbel 4A-4B

8:00AM A7.00001 Magneto-optical evidence of double exchange in a percolating lattice¹. LEONARDO DEGIORG, ETH Zurich — Because of the potential technological applications, materials exhibiting colossal magnetoresistive (CMR) effects are of high current interest in solid state physics. Europium hexaboride (EuB₆) and the well known manganites, for which the onset of ferromagnetism is accompanied by a dramatic reduction of the electrical resistivity, are primary examples, that have intensively been studied. We concentrate on the series of cubic Eu₁₋ₓCoₓB₆, which displays interesting correlations between magnetic, transport and optical properties. Substituting Eu by Co in ferromagnetic EuB₆ leads to a percolation limited magnetic ordering. We present and discuss magneto-optical data of the Eu₁₋ₓCoₓB₆ series, based on measurements of the reflectivity R(ω) from the far infrared up to the ultraviolet, as a function of temperature and magnetic field. Via the Kramers-Kronig transformation of R we extract the complete absorption spectra of samples with different values of x. The change of the spectral weight in the Drude component by increasing the magnetic field agrees with a scenario based on the double exchange model, and suggests a crossover from a ferromagnetic metal to a ferromagnetic Anderson insulator upon increasing Co-content at low temperatures. This work appeared in Phys. Rev. Lett. 96, 016403 (2006)


8:36AM A7.00002 Exploring Competing Interactions in the Hexaborides with Field- and Pressure-Tuned Optical Spectroscopy. S. COOPER, University of Illinois at Urbana-Champaign — No abstract available.
9:12AM A7.00003 Disentangling Surface and Bulk Electronic Structures of EuB$_6$. 1 JONATHAN DENLINGER 2, Lawrence Berkeley National Laboratory — By means of angle-resolved photoemission, the surface and bulk electronic structures of UHV-cleaved ferromagnetic hexaboride EuB$_6$ have been disentangled to reveal both a variable density surface 2D electron gas and an exchange splitting of the boron p-bands below the bulk ferromagnetic ordering temperature of the localized Eu 4f moments. Surface-slab LDA calculations find (i) a distinct surface-related band residing in the bulk-projected bandgap along X-M, (ii) a 2D X-point electron pocket, and (iii) energy-shifted surface-atom Eu 4f states resulting from an electric dipole at the highly ionic surface. These surface-related features manifest in experiment as time dependent effects, the filling of a small X-point electron pocket of Eu 4d-character, correlated to changes in the overall B-p band structure and a splitting of the Eu 4f states. The time-dependent behavior is explained in terms of clustering of mobile surface Eu atoms on the freshly cleaved surface. Understanding and control of these surface effects then allows the bulk electronic structure to be discerned, including a pinning of the Fermi level to the bulk X-point valence band maximum and the magnitude of the valence band exchange splitting below $T_c$.

1Supported by the U.S. DOE at the Advanced Light Source (DE-AC02-05CH11231) and the U.S. NSF at U. of Michigan (DMR-0302825).

9:48AM A7.00004 Double exchange model and magnetic polarons in Eu-based hexaborides. VITOR M. PEREIRA, Boston University and University of Porto — In this presentation, important details of the Double Exchange model at low densities and their pertinence to the physics of ferromagnetic hexaborides will be addressed. After a brief survey of some key experiments and signatures of these compounds, it will be shown that in such systems, where itinerant electrons at extremely reduced densities interact with a dense local spin subsystem, effects of Anderson localization are paramount, providing a consistent picture of the remarkable and unusual response of materials like Eu$_1$-$x$Ca$_x$B$_6$ in magnetic, optical and transport measurements. In this context we will show how one can understand the blue shift in the plasma frequency, the enhancement of carrier density and the CMR effect upon entering the ferromagnetic phase of EuB$_6$ as effects stemming from Anderson localization mechanisms. We will provide an interpretation for the metal insulator transition that occurs upon doping, under the light of recent magneto-optical experiments. In addition, the region of stability of magnetic polarons in the low density Double Exchange Model is discussed, and shown to be consistent with experimental hints of a polaronic phase mediating the PM-FM transition in the vicinity of $T_C$.

10:24AM A7.00005 Magnetic polarons in EuB$_6$ and other low carrier density ferromagnets. MARIA CALDERON, Ins. Ciencia de Materiales de Madrid (CSIC) and Condensed Matter Theory Center (University of Maryland) — Magnetic polarons are formed in systems with low carrier density and large local exchange coupling between the spin background and the spin of the carrier. Magnetic polarons can be free, as in manganese pyrochlores, or bound by Coulomb interaction to impurities in the lattice, as in diluted magnetic semiconductors. EuB$_6$ is a likely candidate for the formation of magnetic polarons as revealed by spin flip Raman scattering and muon-spin rotation measurements. I will give a general perspective on magnetic polarons with a focus on EuB$_6$ and other low density ferromagnets. In such a system, the low density Double Exchange Model is discussed, and shown to be consistent with experimental hints of a polaronic phase mediating the PM-FM transition.

Monday, March 5, 2007 8:00AM - 11:00AM — Session A16 DCMP GMAG: Ab-initio Theory of Spin Dependent Properties Colorado Convention Center Korbel 4F

8:00AM A16.00001 Electronic structure theory of wide gap dilute magnetic semiconductors. LINHUI YE, A.J. FREEMAN, Northwestern University — The recent exciting reports that wide gap semiconductors, notably ZnO, TiO$_2$ and GaN, when doped with transition metal elements, may have $T_c$'s that are higher than room temperature have attracted great interest. When interpreted with care, highly precise first principles FLAPW calculations such as used here are now providing insights into the nature of their strong ferromagnetism (FM). Here, we present an analysis to the electronic structures of several typical wide gap DMS's and illustrate how first principles calculations can lead to correct predictions of their magnetic properties for both Cr:TiO$_2$ and Mn:GaN. The results demonstrate the importance of defect compensation in the determination of the magnetism. A comparison between Mn:ZnO and Co:ZnO highlights the fundamental difference in their electronic structures which explains why their FM is dependent on carriers of different polarity. Correct predictions of their magnetism are found to be due to the correct treatment of the LDA band gap problem. Finally, we provide semi-quantitative discussions of Co doped TiO$_2$, and illustrate why it is highly non-trivial to fully explain its FM based on first principles calculations.

1Supported by NSF through its MERSEC at NU

8:12AM A16.00002 Spin-driven transition metal clustering in the wide-gap ferromagnetic semiconductor Cu$_2$O:Co$_{1-x}$CA16.00002. HANNES RAEBIGER, STEPHAN LANY, ALEX ZUNGER, National Renewable Energy Lab., Golden CO 80401 — Cu$_2$O is a prototype material for p-type transparent conductive oxides, and a host material for diluted magnetic semiconductors. Using local density-functional supercell calculations we study (i) the origin of p-type behavior of pure Cu$_2$O, and (2) the short and long range magnetic interactions of Co atoms substituting Cu. We find that (i) Cu vacancies produce holes, which O vacancies are not able to destroy thus explaining the natural p-type, (ii) a single Co induces a fully occupied and localized level near midgap. This would suggest Co–Co magnetic interactions to be weak because there is no energy gain in magnetic coupling. Nevertheless, (iii) we find that Co–Co pairs lead to a huge ferromagnetic stabilization energy and binding energy, both of around 0.5 eV/pair. This dimerization is accompanied by strong lattice relaxation and symmetry breaking together with level splitting. Both clustering and ferromagnetism are caused by the fact that the bonding states of the previously unoccupied levels become occupied and are lower in energy relative to the antibonding levels of previously occupied levels. Such binding is allowed only for Co atoms with the same spins, leading to ferromagnetism (albeit short ranged).

3Supported by DARPA under NREL contract No. DE-AC36-99GO10337

8:24AM A16.00003 Mechanism of ferromagnetism in wide band gap semiconductors. PRIYA MAHADEVAN, S.N. Bose National Centre for Basic Sciences — Several wide bandgap semiconductors/oxides doped with small concentrations of transition metal impurities have been found to exhibit ferromagnetism at temperatures higher than room temperature. As the typical dopant concentrations are far below the percolation threshold associated with nearest neighbor cation coupling, a picture of ferromagnetism has been proposed which attributes an important role played by the intrinsic defects which are found in these materials. We have considered several examples of the most common defects found in GaN and ZnO, and examined how their presence modifies ferromagnetism. Some defects, such as Ga-vacancies in GaN favor strongly spin polarised configurations with exchange splittings as large as 1 eV. However, the exchange splittings are quenched if the defect induced levels are below the transition-metal induced levels. We consider various scenarios for the location of the defect induced levels and the transition metal levels and identify the regime of defect enhanced ferromagnetism and examine various features of this regime.
structures made of spherical L1\textsubscript{0} quantum-mechanically whilst dealing with a large number of atoms. In this presentation, we show a direct quantum mechanical simulation of magnetic nanostructures with 1D geometry. We present equilibrium interatomic distances, spin- and orbital moments, and the values of MAE. Across the series the easy axis interaction, revealing its utter importance for magnetism in these structures. The calculations were performed with the one-dimensional (1D) version of the full-potential linearized augmented plane-wave (FLAPW) method. The new 1D-FLAPW scheme [1] is extremely fast and allows a natural treatment of structures with 1D geometry. We present equilibrium interatomic distances, spin- and orbital moments, and the values of MAE. Across the series the easy axis of magnetization oscillates between two possible directions: perpendicular and along the wire axis. The largest values of the MAE occur at the end of the series. Giant values of 30-100 meV/atom can be obtained upon stretching of 4d- and 5d-TM wires. Certain chains change the magnetization direction upon wire stretching, opening new perspectives in controlling the spin-dependent ballistic conductance in these structures [2]. [1] Y.Mokrousov et al., Phys. Rev. B 72, 045402 (2005), [2] Y.Mokrousov et al., Phys. Rev. Lett. 96, 147201 (2006)
10:00AM A16.00011 Qualitative aspects of magnetism formation in Gd and its compounds. KIRILL BELASHCHENKO, University of Nebraska-Lincoln, VLADIMIR ANTROPOV, GERMAN SAMOLOYUK, Ames Laboratory — Using highly precise full-potential electronic structure calculations, we study the formation of magnetism in gadolinium. By manipulating the 4f-shell magnetic moments in a large supercell, the interplay between on-site and off-site contributions to the spin polarization of valence electrons is analyzed. Qualitative features of exchange coupling are discussed, and the limitations of model RKKY-like approaches are demonstrated. We also analyze the magnetization density distribution in ferromagnetichcp Gd which, unlike transition-metal ferromagnets, shows a strongly inhomogeneous, directional structure in the interstitial region. The qualitative features revealed in this study are very generic, and we discuss their relevance to other rare-earth elements and their compounds.

10:12AM A16.00012 First-principles Calculation of Atom-scale Magnetic Interaction, BARBARA JONES, IBM Almaden Research Center, San Jose, CA 95120-6099, CHIUNG-YUAN LIN, IBM Almaden Research Center, San Jose, CA 95120-6099 and the Center for Probing the Nanoscale, Stanford University, Stanford, CA 94305 — The advance of manipulating atoms on surfaces by STM has made it possible to study atomic magnetism. It has been shown that STM can build chains of magnetic atoms and measure magnetic excitation of such chains [1]. This new technique has potential application to explore the limits of magnetic data storage. By engineering the energy required to flip the collective orientation of a small number of magnetically coupled atoms, we have applied GGA+U to determine the atomic spin and calculate the exchange coupling, J (several meV) for Mn chains on a CuN/Cu(100) surface. Our spin-density analysis shows that Mn atoms in such a surface preserve their atomic spins S=5/2. To demonstrate the potential to engineer the coupling between atomic spins, we calculate the J's for the Mn dimers atop Cu atoms and atop N in the CuN layer, and find the Cu-site dimer has its J twice as large as the N-site. The local structures of the Mn dimers on these two sites determined by relaxation account for this difference in J. The charge transfers between Mn and its neighboring atoms are also calculated. [1] C. F. Hirjibehedin, C. P. Lutz, A. J. Heinrich, Science 312, 1021 (2006).

10:24AM A16.00013 Ab-initio determination of magnetic properties of Fe-Co nanoclusters on Cu(100). JAN ZABLOUDIL, CORINA ETZ, Center for Computational Materials Science, TU-Vienna, BENICE LAZAROVITS, BALAZS UJFALUSY, Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, LASZLO SZUNYOGH, Center for Applied Mathematics and Computational Physics, Budapest University of Technology and Economics, PETER WEINBERGER, Center for Computational Materials Science, TU-Vienna — By making use of the fully-relativistic screened Korringa-Kohn-Rostoker method supplemented by the embedded cluster method the spin and orbital magnetic moments as well as the magnetocrystalline anisotropy energy (MAE) of Fe-Co nanoclusters of different sizes are explored as a function of the cluster composition. The MAE and magnetic moments are found to vary strongly in dependence on the concentration of Fe and Co atoms as well as on specific arrangements of atoms within the clusters. Consequentially the easy magnetization axis can be tuned by controlling the cluster composition. In contrast to clusters of a pure material there exist additional contributions to the anisotropy in the surface plane due to the two different atomic species.

10:36AM A16.00014 Magnetism of small Co clusters as a probe of ab initio theory, CLAUDIA TROPAREVSKY(*), The University of Tennessee and Oak Ridge National Laboratory, FERNANDO REBOREDO(†), Oak Ridge National Laboratory, ADOLFO EGUILUZ(*), The University of Tennessee and Oak Ridge National Laboratory — We report ab initio calculations of the electronic and magnetic properties of small Co clusters. We performed pseudopotential-based and all-electron calculations. In view of the “unwritten theorem” that electron localization enhances the electronic correlations, we have also considered the LDA+U functional, which is tailored for the strong-correlation problem associated with, e.g., partially-filled d shells. As a result of the weak dependence of the electronic structure on the calculated magnetic moment, the latter is very sensitive to the method employed. Thus, the magnetic moments obtained in the all-electron and pseudopotential calculations are quite different. Furthermore, the on-site Hubbard U enhances the magnetic moment significantly. The available experimental data for the magnetic moment of small clusters [Billas et al., Science 265, 1682 (1994)] are consistent with this enhancement. Additional Stern-Gerlach measurements for smaller clusters would, in combination with our ab initio results, constitute a direct determination of the U for these prototypes of correlated-electron behavior. (*) Supported by NSF Grant ITR DMR-0219332 (†) Managed by UT-Battelle, for the U.S. DOE under contract DE-AC05-00OR22725

10:48AM A16.00015 Non-collinear magnetism in Permalloy (Ni$_{80.8}$Fe$_{19.2}$). MARKUS EISENBACK, DON NICHOLSON, G. MALCOLM STOCKS, Oak Ridge National Laboratory — Permalloy is an important material in a wide variety of magnetic systems, most notably in GMR read-heads. However, despite this great interest its properties are not fully understood. For an in depth analysis of important physical properties as e.g. electric transport or magnetic anisotropy a detailed understanding of the distribution of magnetic moments on an atomic level is necessary. Using our first principles Locally Self-consistent Multiple Scattering (LSMS) method we calculate the magnetic ground state structure for a large super-cell model of Permalloy. Our code allows us to solve both the usual non-relativistic Schrödinger equation as well as the fully relativistic Dirac equation and to find the exchange coupling, J (several meV) for Mn chains on a CuN/Cu(100) surface. Our spin-density analysis shows that Mn atoms in such a surface preserve their atomic spins S=5/2. To demonstrate the potential to engineer the coupling between atomic spins, we calculate the J's for the Mn dimers atop Cu atoms and atop N in the CuN layer, and find the Cu-site dimer has its J twice as large as the N-site. The local structures of the Mn dimers on these two sites determined by relaxation account for this difference in J. The charge transfers between Mn and its neighboring atoms are also calculated. [1] C. F. Hirjibehedin, C. P. Lutz, A. J. Heinrich, Science 312, 1021 (2006).

Monday, March 5, 2007 8:00AM - 9:48AM – Session A31 DCMP: Cold Fusion I

8:00AM A31.00001 Cold Fusion – An 18 Year Retrospective Short Description, MICHAEL C.H. MCKUBRE, SRI International, Menlo Park, CA 94025 — 18 years after the APS voted to refute the reality of Cold Fusion in Baltimore, it is appropriate to consider what has changed. Who was right? We will review the current state of knowledge from the perspective of what we know now compared to what we knew then. Discussion will be made of various avenues of research that we have followed from the original Fleischmann Pons proposal: some failed, some unresolved and some successful.

8:12AM A31.00002 Production of High Energy Particles Using the Pd/D Co-Deposition Process, PAMELA A. MOSIER-BOSS, STANISLAW SZPAK, FRANK E. GORDON, SPAWAR Space Systems Center, San Diego — Using the Pd/D co-deposition technique, we have obtained evidence (i.e., heat generation, hot spots, mini-explosions, radiation, and tritium production) suggestive that nuclear reactions can and do occur within the Pd lattice. It was found that these reactions are enhanced in the presence of either an external electric or magnetic field. SEM analysis of the cathodes shows morphological features suggestive of localized melting of the palladium. EDX analysis of these features show the presence of new elements which result from transmutation. To verify that these new elements are indeed nuclear in origin, experiments have been conducted using CR-39 detectors, a commonly used etch-track detector for recording the emission of high energy particles such as alphas and protons. When the co-deposition reaction was conducted in either an external electric or magnetic field, numerous tracks due to high energy particles were clearly observed on the CR-39 detector in those areas where the cathode is in direct contact with the detector.


8:24AM A31.00003 Accuracy of Cold Fusion Calorimetry, MELVIN H. MILES, Department of Chemistry, University of LaVerne, LaVerne, CA 91750 (mmiles@ulv.edu), MARTIN L. FLEISCHMANN, Fellow of the Royal Society, Bury Lodge, Duck Street, Tisbury, Salisbury, Wilts., SP36LJ, U.K. — The cold fusion controversy centers on the precision and accuracy of the calorimetric systems used to measure excess enthalpy generation. For open, isoperibolic calorimetric systems, there is no true steady state during D2O-LiOD electrolysis. Exact calorimetric measurements, therefore, require modeling by a differential equation that accounts for all heat flow pathways into and out of the calorimetric systems. The improper use and misunderstanding of this differential equation is a major source of confusion concerning cold fusion calorimetric measurements. The use of a platinum cathode as a control showed that excess power due to the controversial recombination effect was measurable at 1.1 plus or minus 0.1 mW. Theoretical calculations using Henry’s Law and Fick’s Law of Diffusion yield approximately 1 mW for this effect due to oxygen reduction at the cathode. Palladium-boron alloy materials prepared at the Naval Research Laboratory have shown a remarkable ability to produce excess power effects in the range of 100 to 400 mW. The excess power increased to over 9000 mW during the final boil-off phase in one experiment.

8:36AM A31.00004 Resonant Interaction, Approximate Symmetry, and Electromagnetic Interaction (EMI) in Low Energy Nuclear Reactions (LENR), SCOTT CHUBB, Research Systems, Inc, 9822 Pebble Weigh Ct., Burke, VA 22015-3378 — Only recently (talk by P.A. Mosier-Boss et al, in this session) has it become possible to trigger high energy particle emission and Excess Heat, on demand, in LENR involving PdD. Also, most nuclear physicists are bothered by the fact that the dominant reaction appears to be related to the least common deuteron(d) fusion reaction, d+d→α+γ. A clear consensus about the underlying effect has also been illusive. One reason for this involves confusion about the approximate (SU2) symmetry: The fact that all d+d fusion reactions conserve isospin has been widely assumed to mean the dynamics is driven by the strong force interaction (SFI), NOT EMI. Thus, most nuclear physicists assume: 1. EMI is static; 2. Dominant reactions have smallest changes in incident kinetic energy (T); and (because of 2), d+d→α+γ is suppressed. But this assumption has a stronger form of SU2 symmetry than is present: d+d→α+γ reactions are suppressed not because of large changes in T but because the interaction potential involves EMI, is dynamic (not static), the SFI is static, and because the two incident deuterons must have approximate Bose symmetry and vanishing spin. A generalization of this idea involves a resonant form of reaction, similar to the de-excitation of an atom. These and related (broken gauge) symmetry EMI effects on LENR are discussed.

8:48AM A31.00005 1.6 MHz Sonofusion Model and Measurement, ROGER S. STRINGHAM, First Gate Energies PO Box 1230, Kilauea, HI 96754 — Years of data collected by First Gate, involving various sonofusion systems, gains some support from recent extrapolations of hot fusion research. Consider the 10^4 kHz of the high density low energy jet plasma of deuterons that originates from the collapse of the transient cavitation bubble (TCB), in D2O that implants a target foil. And compare it to the jet plasma of Tokamak type plasmas with all their stability problems. Also consider the relevance of the impeding wire technology where the magnetohydrodynamic pressures exceed the crystal forces that bind atoms in wire conductors and inertial confinement fusion (ICF). Applying this developed technology to the TCB jet plasmas of sonofusion makes the transition between hot and “cold” fusion more attractive. Our measurements show there is no long range radiation (gammas or neutrons) and 4He is the fusion product. These problems are addressed via coherence in the implanted high density transient deuteron Bosons (and proton Fermions) clusters in the heat producing target.

9:00AM A31.00006 Selective Resonant Tunneling through Coulomb Barrier by Confined Particles in Lattice, X.Z. LI, Q.M. WEI, B. LIU, Department of Physics, Tsinghua University, Beijing 100084, China — In 1993, Kasagi discovered the anomalous yield of 3 deuteron fusion reaction while searching the branching ratio of d+d fusion at low energy. In 1995-1997, Takahashi carefully studied this anomalous yield of 3 deuteron fusion reaction again. Distinct from the early Kasagi’s study, Takahashi studied another 3 deuteron fusion channel: i.e. d+d+d→t (4.75MeV) + 3He (4.75MeV). Because only 2 nuclear products were emitted from this reaction channel, triton and helium-3 were clearly identified by their energy. From this information, Takahashi estimated the life-time of the 2 deuteron (2-d) resonance. It was in the order of 10^5 seconds. In this paper, selective resonant tunneling model was applied to calculate the life-time of this 2-d resonance inside the deuterated titanium. A square-well is assumed for the nuclear potential.

9:12AM A31.00007 Low Energy Nuclear Reactions: 2007 Update, STEVEN B. KRIVIT, New Energy Times, 11664 National Blvd. #142, Los Angeles, CA 90064 — This paper presents an overview of low energy nuclear reactions, a subset of the field of condensed matter nuclear science. Condensed matter nuclear science studies nuclear effects in and/or on condensed matter, including low energy nuclear reactions, an entirely new branch of science that gained widespread attention and notoriety beginning in 1989 with the announcement of a previously unrecognized source of energy by Martin Fleischmann and Stanley Pons that came to be known as cold fusion. Two branches of LENR are recognized. The first includes a set of reactions like those observed by Fleischmann and Pons that use palladium and deuterium and yield excess heat and helium-4. Numerous mechanisms have been proposed to explain these reactions, however there is no consensus for, or general acceptance of, any of the theories. The claim of fusion is still considered speculative and, as such, is not an ideal term for this work. The other branch is a wide assortment of nuclear reactions that may occur with either hydrogen or deuterium. Anomalous nuclear transmutations are reported that involve light as well as heavy elements. The significant questions that face this field of research are: 1) Are LENRs a genuine nuclear reaction? 2) If so, is there a release of excess energy? 3) If there is, is the energy release cost-effective?
9:24AM A31.00008 Physics in a Many-Centered Environment. TALBOT A. CHUBB, Physicist Consultant, 5023 N. 38th St., Arlington, VA 22207 — Physics in a many-center environment was born as the electron physics of metals. Electrons moving from the electrolyte of a battery to anode metal become quasi-particles with a many-centers geometry. The Ion Band State Theory of cold fusion assumes that a fraction of the deuterons in PdD$^+$ reconfigure to a many-centers geometry. Many-center geometry seems to apply to deuteron populations in nano-metal crystals as studied by Arata and Zhang, to Bloch-sensitive nuclei created in Iwamura’s permeation studies, to the metastable nuclei forming alpha shower flakes as discovered by Oriani and Fisher and reproducibly produced by F. Mosier-Boss.

2 T.A. Chubb, “Many-Centers Nuclei,” submitted to Infinite Energy

9:36AM A31.00009 Heat Produced During Electrolysis with a Tubular Pd Cathode. WU-SHOU ZHANG, JOHN DASH, QIONGSHU WANG, Low Energy Nuclear Laboratory, Portland State University, Portland, OR 97207-0751 — An explosion occurred during electrolysis of heavy water with a tubular Pd cathode from the same batch as used as the anode in the above experiments. The Pd tube containing the electrolyte was placed in a Seebeck envelope calorimeter which is capable of accurate heat measurements. Data was obtained first from a three cm length of the tube on one end, and then from a three cm length on the opposite end. There were no explosions, but both ends of the tube produced continuous excess thermal power (356 mW +/- 11 mW maximum). In addition there were 39 heat bursts (1.1 W maximum) from the first end during 201 hours of electrolysis and 58 heat bursts (1 W maximum) during 443 hours of electrolysis from the opposite end of the tube. The period of the heat bursts ranged from a few minutes to 3.3 hours. Data on the topography and microchemical composition of the tube surface before and after electrolysis will also be presented.


Monday, May 5, 2007 11:15AM - 2:15PM - Session B3 DCMP: Phonons and Magnetic Frustration in Pyrochlores Colorado Convention Center Korbel 2A-3A

11:15AM B3.00001 Quenching ground state degeneracy in pyrochlore antiferromagnets. DORON BERGMAN, UCSB — The classical pyrochlore antiferromagnet (AFM) is considered the “most” geometrically frustrated system. Classically, this leads to the absence of any ordering transition at non-zero temperature, even in an applied magnetic field. We describe several mechanisms by which the ground state degeneracy can be split by fluctuations or other effects. We first consider quantum fluctuations, which may lead to the formation of a novel spin-liquid state or complex magnetic ordering. By deriving an effective Hamiltonian, we determine the quantum ground states for different values of spin $s$, resolving some of the ambiguities in existing large-$s$ spin-wave treatments. A quantitative application to recent experiments on the spinel chromites, ACr$_2$O$_4$ (A=Cd, Hg) shows that for the relevant $s = 3/2$ the quantum effects are too weak to explain the observed ordering and the existence of a very robust magnetization plateau in a field. We then consider the role of a finite magnetic field. The plateau is markedly suppressed by both the plateau saturation field was used as the field on the plateau. This in a Seebass is confirmed by recent neutron scattering and x-ray scattering experiments (S. H. Lee et al.). The same model applied to zero magnetic field predicts a reduced but still large ground state degeneracy, including the states observed in both the Cd and Hg materials. This is consistent with the dominance of spin-lattice interactions, with weak additional effects determining the low field magnetic ordering.

11:51AM B3.00002 Heisenberg antiferromagnet on the pyrochlore lattice: order from distortion. OLEG TCHERNYSHYOV, Johns Hopkins University — The Heisenberg antiferromagnet on the pyrochlore lattice is an example of a highly frustrated system with a large degeneracy of the ground state. The classical model with nearest-neighbor interactions shows no signs of magnetic order down to very low temperatures. The quantum analog, with short enough spins, was considered a prime candidate for a quantum-disordered ground state, such as a valence-bond liquid or solid. At the same time, the large degeneracy makes this magnet susceptible to a variety of nominally small perturbations. A spin-lattice coupling leads to a spin-Peierls-like distortion of the lattice. In contrast to spin chains, the spin-Peierls distortion in a pyrochlore antiferromagnet occurs for any spin length $S$ remaining robust even in the classical limit. A recent experimental characterization of the $S = 3/2$ prototype CdCr$_2$O$_4$ [1] provided a test for the theoretical model. This antiferromagnetic spinel exhibits a tetragonal lattice distortion with an elongated unit cell $a = b < c$ and a weakly incommensurate spiral magnetic order with ordered moments in the $a$ plane and a magnetic Bragg peak at $(0, \delta, 1)$, where $\delta \ll 1$. We show [2] that the observed structural and magnetic orders are consistent with one of the spin-Peierls scenarios described previously. The distortion, caused by an odd phonon doublet $E_u$, breaks the inversion symmetry. The magnetic order is collinear to a first approximation. The broken parity makes the crystal structure chiral. The handedness of the lattice is transferred to the magnetic order resulting in a long-period spiral that agrees in detail with observations.


Supported in part by the NSF Grant No. DMR-0348679

12:27PM B3.00003 Nonlinear optical signatures of the tensor order in Cd$_2$Re$_2$O$_7$. J. STEVEN DODGE, Simon Fraser University — The pyrochlore oxide Cd$_2$Re$_2$O$_7$ undergoes a structural phase transition at $T = 200$ K with an unusual tensor character. The order parameter for this state is two-dimensional, and associated with a phonon mode with $E_u$ symmetry. In magnetically frustrated pyrochlores, magnetoelastic coupling to similar modes can induce fascinating magnetically ordered states. Cd$_2$Re$_2$O$_7$ is nonmagnetic, so it is possible to study the structural instabilities of the pyrochlore lattice in isolation. We have used optical second harmonic generation with polarization sensitivity to resolve an ambiguity in the low-temperature crystal structure, and verify an auxiliary condition on the structure that is implied by the order parameter symmetry. We also show that the temperature-dependence of the order parameter is consistent with thermal occupation of a Goldstone mode that results from the $E_u$ order parameter symmetry. The methodology that we have developed may be applied more widely in characterizing ordered states in matter.

1 Work supported by NSERC; the Canadian Institute for Advanced Research; the Sloan Foundation; the Research Corporation; and the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, US Department of Energy.
1:03PM B3.00004 Frustrated and Satisfied Ground States in Pyrochlore Antiferromagnet \( \text{Tb}_2\text{Ti}_2\text{O}_7 \)\(^1\), BRUCE GAULIN, McMaster University — The Rare-Earth Titanates have been a playground for the physics of geometrical frustration, as magnetic rare earth sites can be arranged on the pyrochlore lattice, a network of corner-sharing tetrahedra. This leads to exotic low temperature properties. Spins in the pyrochlore lattice have macroscopic ground state degeneracy, that leads to frustrated magnetic interactions.\(^1\) This talk will focus on a quick review of several novel properties found in spinels, such as the spin liquid state in \( \text{ZnCr}_2\text{O}_4 \), the 3D spin-Peierls transition in \( \text{ZnCr}_2\text{O}_4 \), the spin-orbital coupling in \( \text{ZnV}_2\text{O}_4 \), and the heavy fermionic behaviors in \( \text{LiV}_2\text{O}_4 \). A discussion will follow on our recent neutron and X-ray scattering works on \( \text{ACr}_2\text{O}_4 \) (A=Cd, Hg). We will show the 3D spin-Peierls transition in \( \text{CdCr}_2\text{O}_4 \) is different from that observed in \( \text{ZnCr}_2\text{O}_4 \), and that the magnetic field-induced half-magnetization plateau state in \( \text{HgCr}_2\text{O}_4 \) has the \( \text{P4}_3\text{2} \) symmetry. Our results provide direct tests of theoretical models proposed to understand the complex behaviors of the Heisenberg pyrochlore antiferromagnets. A quantum spin pyrochlore system will also be discussed.

\(^{1}\)In collaboration with S. Dunsiger, J. Gardner, K. Rule, J. Ruff, P. Clancy, J. Copley, Y. Qiu

1:39PM B3.00005 Neutron scattering studies of magnetic pyrochlores, SEUNG-HUN LEE, University of Virginia — The pyrochlore antiferromagnets in which spins interact in a network of corner-sharing tetrahedra have macroscopic ground state degeneracy, that leads to exotic low temperature properties. Spinels \( \text{AB}_2\text{O}_4 \) realize the pyrochlore lattice if the B ions couple antiferromagnetically. This talk will start with a quick review of several novel properties found in spinels, such as the spin liquid state in \( \text{ZnCr}_2\text{O}_4 \), the 3D spin-Peierls transition in \( \text{ZnCr}_2\text{O}_4 \), the spin-orbital coupling in \( \text{ZnV}_2\text{O}_4 \), and the heavy fermionic behaviors in \( \text{LiV}_2\text{O}_4 \). A discussion will follow on our recent neutron and X-ray scattering works on \( \text{ACr}_2\text{O}_4 \) (A=Cd, Hg). We will show the 3D spin-Peierls transition in \( \text{CdCr}_2\text{O}_4 \) is different from that observed in \( \text{ZnCr}_2\text{O}_4 \), and that the magnetic field-induced half-magnetization plateau state in \( \text{HgCr}_2\text{O}_4 \) has the \( \text{P4}_3\text{2} \) symmetry. Our results provide direct tests of theoretical models proposed to understand the complex behaviors of the Heisenberg pyrochlore antiferromagnets. A quantum spin pyrochlore system will also be discussed.

Monday, March 5, 2007 11:15AM - 2:15PM – Session B7 DCMP: Emergent Patterns in Geophysical Processes Colorado Convention Center Korbel 4A-4B

11:15AM B7.00001 Dynamics of precipitation pattern formation at geothermal hot springs\(^1\), NIGEL GOLDENFELD, University of Illinois at Urbana-Champaign — The spectacular terraced landscape at geothermal hot springs is a world-wide phenomenon, shown here to arise from the nonlinear interplay between turbulent fluid transport and precipitation dynamics. The system is modeled successfully using a discrete space-time model, justified both from renormalization group considerations and our experience modeling phase transition kinetics in condensed matter systems. A variety of scaling laws are predicted and compared with field observations.

\(^{1}\)This work was supported by NSF Grant NSF-EAR-02-21743

11:51AM B7.00002 Scaling in Columnar Joints\(^1\), STEPHEN MORRIS, University of Toronto — Columnar joints is a fracture pattern common in igneous rocks in which cracks self-organize into a roughly hexagonal arrangement, leaving behind an ordered colonnade. We report observations of columnar jointing in a laboratory analog system, desiccated corn starch slurries. Using measurements of moisture density, evaporation rates, and fracture advance rates, we suggest an advective-diffusive system is responsible for the rough scaling behavior of columnar joints. This theory explains the order of magnitude difference in scales between jointing in lavas and in starches. We investigated the scaling of average columnar cross-sectional areas in experiments where the evaporation rate was fixed using feedback methods. Our results suggest that the column area at a particular depth is related to both the current conditions, and hysteretically to the geometry of the pattern at previous depths. We argue that there exists a range of stable column scales allowed for any particular evaporation rate.

\(^{1}\)Work done with Lucas Geohring and Zhengquan Lin

12:27PM B7.00003 How the Icicle Got Its Shape, MARTIN SHORT, University of Arizona — The growth of icicles is considered as a free-boundary problem. A synthesis of atmospheric heat transfer, geometrical considerations, and thin-film fluid dynamics leads to a nonlinear ordinary differential equation for the shape of a uniformly advancing icicle, the solution to which defines a parameter-free shape which compares very favorably with that of natural icicles. Away from the tip, the solution has a power-law form identical to that recently found for the growth of stalactites by precipitation of calcium carbonate. This analysis thereby explains why stalactites and icicles are so similar in form despite the vastly different physics and chemistry of their formation.

1:03PM B7.00004 Snow spikes: formation of laboratory penitentes, M. D. BETTERTON, University of Colorado — Spike-shaped structures are produced by light-driven ablation in very different contexts. Penitentes 1-4 m high are common on Andean glaciers, where their formation changes glacier dynamics and hydrology. Laser ablation can produce cones 10-100 microns high with a variety of proposed applications in materials science. We report the first laboratory generation of centimeter-scale snow and ice penitentes. Systematically varying conditions allows identification of the parameters controlling the formation of ablation structures. We demonstrate that penitente initiation and coarsening require cold temperatures, so that ablation leads to sublimation. Once penitentes have formed, further growth of height can occur by melting. The penitentes initially appear as small structures (3 mm high) and grow by coarsening to 1-5 cm high. Our results are an important step towards understanding ablation morphologies.

1:39PM B7.00005 Triboelectrification and Razorbacks: Geophysical Patterns Produced in Dry Grains, TROY SHINBROT, Rutgers, The State University of New Jersey — No abstract available.

Monday, March 5, 2007 11:15AM - 2:15PM – Session B9 DCMP: Superconductivity: Currents and Vortex Dynamics Colorado Convention Center Korbel 1D
11:15AM B9.00001 Critical current density distribution in YBCO coated conductors measured with a “magnetic knife”

JENS HANISCH, STEPHEN P. ASHWORTH, FRED M. MUELLER, YATES COULTER, VLADIMIR MATIAS.

Superconductivity Technology Center, Los Alamos National Laboratory — We present a simple and straightforward tool for investigating the spatial Jc distribution in YBCO coated conductors. The samples were prepared by co-evaporation and PLD on IBAD and RABiTS templates. The tool we have used is a “magnetic knife” [1] consisting of several Nd2Fe14B permanent magnets in close proximity to the superconducting tape. A 200 µm wide zone of low magnetic field ΔB is embedded in a background field of around 600 mT. This region is scanned across the sample, in the direction perpendicular to the direction of tape current flow. The critical current for each position is measured with a four-point technique at 75 K (liquid N2 at ambient pressure). The raw data are deconvoluted with a Fourier inversion method. Several techniques for obtaining the magnetic field distribution in the magnetic knife (simulations and measurements) will be compared and discussed. Finally, differences in the current distributions for different coated conductor samples will be discussed. [1] ten Haken et al., Physica C 334, 163 (2000)

11:27AM B9.00002 Testing the limits for critical currents in YBa2Cu3O7 films

LEONARDO CIVALE, BORIS MAIOROV, SCOTT BAILY, HONGHUI ZHOU, FRANK HUNTE, IGOR USOV, STEPHEN FOLTYN, TERRY HOLESINGER, QUANXI JIA. Superconductivity Technology Center, LANL, Los Alamos, NM, JUDITH MACMANUS-DRISCOLL. Dept. of Materials Science, University of Cambridge, UK, HAIYAN WANG, Texas A & M University, College Station, TX — Vortex pinning in YBa2Cu3O7 films can be very strong. At low temperatures and in the absence of applied magnetic field (H), critical current densities Jc of about 20% of the depairing limit have been obtained. This is as high as the best achieved in commercial Nb-based superconducting wires after decades of optimization. Remarkably, similar Jcs are attained in YBa2Cu3O7 films grown by various methods that produce vastly different nanostructures, suggesting that perhaps we are close to an effective Jc limit regardless of the details of the pinning mechanisms. In contrast, the different types of pinning centers (either naturally occurring or artificially introduced by material nanoengineering) produce distinctively different Jc behavior as a function of H strength and orientation. I will present a comparison of pinning mechanisms in YBa2Cu3O7 films and will analyze the possibilities of further improvements.

11:39AM B9.00003 Irreversibility line of YBa2Cu3O7 films as a function of angle and field up to 50 Tesla

S.A. BAILY, B. MAIOROV, F. HUNTE, H. ZHOU, S.R. FOLTYN, Q.X. JIA, L. CIVALE. Superconductivity Technology Center, LANL, Los Alamos, NM, F.F. BALAKIREV, M. JAIME. National High Magnetic Field Laboratory, LANL, Los Alamos, NM — Studying the irreversibility line (resistivity=0) in high-temperature superconductors requires a method to study vortex properties all the way to the vortex solid-liquid transition. We have used low current transport measurements to study the irreversibility line of YBa2Cu3O7 films in fields up to 50 T. Electronic mass anisotropy can describe most of the angular dependence, but fails to account for deviations along the crystalline axes. Correlated pinning causes a large increase in the irreversibility field along the a–b planes, and a small c-axis peak. Inclusion of Ba2ZrO3 not only adds c-axis correlated defects, but increases the overall irreversibility field and alters the shape of the resistivity vs. magnetic field curve in the liquid state. We will discuss the results in terms of vortex pinning, the corresponding types of phase transitions, micro-structural analysis, and information obtained from critical current measurements.

11:51AM B9.00004 AC current driven vortex dynamics in YBCO thin films and coated conductors

ANDREA LUCARELLI, RAN YANG, GUNTER LUEPKE, College of William and Mary, FRANCESCO GRILLI, Los Alamos National Laboratory, TIMOTHY HAUGAN, GEORGE LEVIN, AIR FORCE RESEARCH LABORATORY a. The effect of an AC current and a static magnetic field on the vortex dynamics in YBa2Cu3O7−δ (YBCO) thin films and coated conductors is studied by time-resolved magneto-optical imaging. Our measurements show that the AC current enables the vortex lattice in the YBCO thin film to reorganize into two coexisting states with different characteristics: a quasi-static state in the sample interior and a dynamic state near the edges. Vortices and re-vortices, induced by the current during the cycle, penetrate from the edges into the sample and interact with the pinned vortices altering the flux lattice. We compare the AC current driven vortex dynamics in YBCO thin films and coated conductors with particular focus on the AC loss characteristics of multifilamentary samples. Finite-element method (FEM) calculations adopting a recently developed method, are used to compute current density, field profiles and AC losses during the cycle. The model assumes a thermal activation of the magnetic field that leads to a nonlinear dependence of the electric field and current density. The FEM calculations show a very good agreement with the measured data.

12:03PM B9.00005 Influence of disorder on the vortex pinning and cutting of YBa2Cu3O7 films

B. MAIOROV, L. CIVALE, Q.X. JIA, H. ZHOU, S.R. FOLTYN, T.G. HOLESINGER. Superconductivity Technology Center, LANL, Los Alamos, NM, S. BAILY, Superconductivity Technology Center and National High Magnetic Field Laboratory, LANL, Los Alamos, NM, H. WANG, Texas A & M University, College Station, TX, J.L. MACMANUS-DRISCOLL, Dept. of Materials Science, University of Cambridge, UK, T.N. HAUGAN, P.N. BARNES, Air Force Research Laboratory, Wright-Patterson Air Force Base, OH — Flux cutting and recombination has been used to explain high critical current densities (Jc) observed in high-temperature superconducting thin films and wires. However, the process is not fully understood. In this work, we investigate the influence of defect density and flux-lattice alignment caused by applied magnetic field H on the applied magnetic field H. However, the effect of different pinning centers has not been studied. We present angular and field Jc studies in FF and VLF configurations and study the effects of random, correlated and extended defects on the Jc of YBa2Cu3O7 films. Results are analyzed in terms of vortex pinning at different vortex cutting mechanisms. We show that pinning greatly influences Jc in FF and VLF, up to the point of obtaining Jc higher than Jc(H = 0) up to magnetic fields as high as 3T.

12:15PM B9.00006 Evolution of the vortex-solid to vortex-liquid melting line

inY1−xPrxBa2Cu3O6.96 and YBa2Cu3O6.5 to 45 tesla

B.J. TAYLOR, M.B. MAPLE. University of California, San Diego — By extending magneto-transport measurements to fields up to 45 tesla, we have been able to examine the vortex glass melting line of Y1−xPrxBa2Cu3O6.96 (x = 0 - 0.4) thin film samples and that of an oxygen deficient YBa2Cu3O6.5 single crystal over an extended temperature range, 0.03 Tc < Tc < Tc, larger than has hitherto been reported. The melting lines are analyzed in the context of the model of Blatter & Ivlev (B&I) [PRL 70, 3021 (1993)] with temperature dependent parameters, ξ, λ, etc. The temperature dependence of the relaxation time of a single vortex flux line, displaced by quantum/thermal fluctuations, is deduced such that the entire melting line of each sample can be fit smoothly by the modified expression of B&I, implying that the physical mechanism responsible for the manner and conditions of the melting of the vortex solid can be described smoothly over the entire temperature — field range. This research was supported by the DOE under Research Grant No. DE-FG02-04ER46105. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by NSF Cooperative Agreement No. DMR-0084173, by the State of Florida, and by the DOE.

12:27PM B9.00007 Vortex pinning in single crystal CaCu6

ULRICH WELP, DANIEL ROSENMANN, RUOBING XIE, DAVID HINKS, HELMUT CLAUS, GORAN KARAPETROV, JOHN SCHLIEUER, WAI-KWONG KWOK, Argonne National Laboratory, Argonne, IL 60439, LISA PAULIUS, Western Michigan University, Kalamazoo, MI 49006 — Crystals of the new graphite intercalation superconductor CaCu6 were synthesized in a liquid transport process in which graphite single crystals are exposed to an eutectic Ca-Li melt at 350 °C. The resulting samples display a sharp superconducting transition at 11.6 K. X-ray diffraction reveals the rhombohedral CaCu6 structure with no indication of graphite second phases. The phase diagram and the vortex pinning properties were determined using magnetization and Hall magnetometry measurements. The irreversibility line for fields applied along the c-axis lies close to the upper critical field and displays down to temperatures of 2 K a linear temperature dependence with a slope of about -230 G/K. An analysis based on the Bean critical state model yields a critical current density of 10^6 A/cm² at 4.5 K and zero field. The effect of particle irradiation on the flux pinning properties of CaCu6 will be presented. This work was supported by the US Department of Energy, BES-Materials Sciences, under Contract DE-AC02-06CH11357.
We thank Superpower Inc. for providing IBAD substrates. ORNL is managed by UT-Battelle, LLC for USDOE under contract DE-AC05-00OR22725.

1:03PM B9.00010 Peak Effect in Polycrystalline Vortex Matter1, IVO DIMITROV, NIKOS DANILIDIS, CHARLES ELBAUM, Brown University, JEFF LYNN, National Institute of Standards and Technology, NCNR, XINSHENG LING, Brown University — The peak effect (PE) in type-II superconductors is believed to mark the transition between a disordered vortex state and a quasi-ordered Bragg glass regime. Some strongly-disordered type-II superconductors, such as the binary alloy V-21at.% Ti, also exhibit “peak effect” at temperatures close to Hc2, despite lack of atomic long-range order and presence of sample composition inhomogeneities. SANS field-cooled measurements on a V-21at.% Ti sample show that both deep in the mixed state and close to the PE transition, there exist no long-range orientationally-ordered vortex lattices (VL’s). The neutron scattering data analysis shows that the diffraction radial widths do not change significantly as a function of field, suggesting that VL states ordered on the scale of μm exist. We conjecture that the “peak effect” in V-21at.%Ti corresponds to the disordering of ordered VL Larkin domains. The V-21at.% Ti peak effect phase diagram is mapped via ac susceptometry. This measurement reveals that the peak effect disappears below a certain field, as has been reported in other superconductors.

1Supported by NSF-DMR 0406626

1:15PM B9.00011 Magnetocaloric Studies of the Peak Effect in Nb1, NIKOS DANILIDIS, IVO DIMITROV, VESNA MITROVIC, CHARLES ELBAUM, XINSHENG LING, Brown University — We report a magnetocaloric study of the peak effect and Bragg glass transition in a Nb single crystal. The thermomagnetic effects due to vortex flow into and out of the sample are measured. The magnetocaloric signature of the peak effect anomaly is identified. It is found that the peak effect disappears in magnetocaloric measurements at fields significantly higher than those reported in previous ac-susceptometry measurements. Investigation of the superconducting to normal transition reveals that the disappearance of the bulk peak effect is related to inhomogeneity broadening of the superconducting transition. The emerging picture also explains the concurrent disappearance of the peak effect and surface superconductivity, which was previously reported in the sample under investigation. Based on our findings we discuss the possibilities of multir critically associated with the disappearance of the peak effect.

1Supported by NSF-DMR 0406626

1:27PM B9.00012 Collapse of the critical state in superconducting niobium1, RUSLAN PROZOROV, Ames Laboratory and Department of Physics & Astronomy, Iowa State University, Ames, Iowa 50011, DANIEL V. SHANTSEV, Department of Physics, University of Oslo, P. O. Box 1048 Blindern, 0316 Oslo, Norway, ROMAN G. MINTS, School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978, Israel — Giant abrupt changes in the magnetic flux distribution in niobium foils were studied by using magneto-optical visualization, thermal and magnetic measurements. Uniform flux jumps and sometimes almost total catastrophic collapse of the critical state are reported. Results are discussed in terms of thermomechanical instability mechanism with different heat removal channels. Video figures are available at: http://www.cmplgroup.ameslab.gov/supermaglab/video/Nb.html

1Supported by NSF Grant DMR-05-53285 and by the Alfred P. Sloan Research Foundation.

1:39PM B9.00013 Analysis of collective pinning and depinning of the flux line lattice in pristine 2H-NbSe2, JONGCHEE LEE, HUI WANG, MICHAEL DREYER, Department of Physics, University of Maryland, College Park, MD 20742, BARRY I. BARKER, Laboratory for Physical Sciences, National Security Agency, 8050 Greenmead Drive, College Park, MD 20740 — Larkin and Ovchinnikov predicted collective pinning of the flux line lattice (FLL) in type II superconductors several decades ago. The collective pinning results from the interplay between strong vortex-vortex interaction and randomly distributed weak pinning centers in a media. The evidence of collective pinning was previously observed at a magnetic field, H, close to Hc2 in current-driven transport experiments on the macroscopic scale. But there still exists a lack of understanding of collective pinning on the microscopic level. In this talk, we show collective pinning and depinning of the FLL in pristine 2H-NbSe2 in a long time series (15 days), measured by a low temperature scanning tunneling microscope. We observed the motion of the FLL within an area of 400 nm x 400 nm, with an initial magnetic field of 0.5 T. The motion was caused by the very slow decay of magnetic field (~ 5 nT/s) in a defective superconducting magnet. The average speed of FLL was ~ 2.5 pm/s, lower than previously reported. Using highly time resolved data, we will further discuss the average direction of motion, the strength of pinning centers in pristine 2H-NbSe2, flux line mass, and the difference between current-driven and field-driven FLL motions.

1:51PM B9.00014 Paramagnetic effect in nano-opal-lead structure, FULIN ZUO, HENGSHENG ZHANG, University of Miami, DI WU, JING SHI, University of California — We report magnetic studies of the paramagnetic effect observed in the superconducting nano-structured opal-lead system. Positive magnetization is clearly observed when the sample is cooled in field. The paramagnetic effect is strongly dependent on the applied field, cooling rate and the background magnetization. The results suggest that the paramagnetic moment is due to flux trapping and the competition between the positive and negative moments due to the temperature dependence of penetration depth.
superconductors. Experimental fact that has not been given a theoretical explanation: instabilities always disappear above some upper threshold field. Our recently developed magnetic instabilities, are known to destroy a metastable critical state and severely detriment performance of SC applications. Several thermo-magnetic models have been proposed to determine conditions under which a superconductor is to undergo a dendritic magnetic avalanche. However, there remains an omnipresent mechanism due to a strong dependence of the critical current on magnetic field $j_c$. We then verify the model in a range of controllably varied $j_c$ values.

**Monday, March 5, 2007 11:15AM - 1:15PM – Session B31 DCMP: Cold Fusion II Colorado Convention Center 401**

**11:27AM B31.00002 Engineering of Condensed Matter Nuclear Physics: Heterodyne Behavior in Condensed Matter Nuclear Systems**, MITCHELL R. SWARTZ, JET Energy, Inc., Wellesley, MA 02481 — Previously, we reported method to semi-quantitatively measure and control tardive thermal power (TTP) which develops long after the termination of electric input power in condensed matter high-deuteron-flux Phusor devices providing (Pt/D2O/Pd; 0.5 cm$^2$) peak excess power ratios circa $2.30^{+/-0.84}$. Now we report one method to improve excess energy using heterodyne CMN systems using both normal and TTD operation - heterodyne operation (that is, hetero for other, and $dyne$ for power). By augmenting the conventional excess energy produced by CMN active systems (normal operation) with the additional energy ("other power") resulting from the time integral of TTP ("heat after death"), the net time-integrated excess energy (output energy beyond that applied as the input energy) is greater than we have previously reported and may be maximized using TTD drive techniques. Initial experiments of heterodyned active samples, capable of excess heat operation at the optimal operating point, have yielded excess energy increases of up to four times beyond that obtained without heterodyned operation.

**11:39AM B31.00003 Maruhn-Greiner Maximum for Confirmation of Low Energy Nuclear Reactions (LENR) via a Compound Nucleus with Double Magic Numbers**, HEINRICH HORA, Department of Theoretical Physics, University of New South Wales, Sydney 2052, Australia (h.hora@unsw.edu.au)

Maruhn-Greiner mechanism. We suggest this phenomenon can be explained by the strong screening of the Maxwellian ds on the degenerate rigid electron background with the swimming electrons at the metal surface or thin film interfaces. The deuterons behave like neutrals at distances of above 2 picometers (pm) and form clusters due to soft attraction in the range of thermal energy; 10 pm diameter clusters can react over long time scales ($10^6$ s) with Pd leading to double magic number compound nuclei $306x126$ decaying via fission to an $A=153$ element distribution.

**11:51AM B31.00004 The Science of Low Energy Nuclear Reactions**, EDMUND STORMS, Energy Case Systems, 2140 Paseo Ponderosa, Santa Fe NM 87501 — The large literature describing the anomalous behavior attributed to cold fusion or low energy nuclear reactions has been critically described in a recently published book. Over 950 publications are evaluated allowing the phenomenon to be understood. A new class of nuclear reactions has been identified that are able to generate practical energy without significant radiation or radioactivity.

**12:03PM B31.00005 Time Resolved, High Resolution Gamma Ray and Integrated Charged and Knock-on Particle Measurements of a Pd:D Co-deposition Cell**, LAWRENCE P.G. FORSLEY, GARY PHILLIPS, JAY KHIEM, JVK Technologies Corporation, 7617 Little River Turnpike Suite 1050, Annandale, VA 22003. PAMELA MOSIER-BOSS, FRANK GORDON, STANISLAW SZPAK, SPAWAR Space Systems Center, San Diego — Time resolved, with a 10 second interval, high resolution gamma ray measurements using a high efficiency cryogenically cooled gamma ray detector have been taken simultaneously with a CR-39 integrating charged particle detector on a series of experiments in conjunction with the Navy SPAWAR Pd:D co-deposition cell. These results include anomalous, coincident, gamma ray emissions from witness materials in the cell in conjunction with the CR-39 data. There is evidence of a variety of knock-on particles as well. The copious data, exceeding 10,000 tracks/mm$^2$, offers a means to distinguish among various condensed matter nuclear science theories.

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1Department of Theoretical Physics, University of New South Wales, Sydney 2052, Australia (h.hora@unsw.edu.au)


12:15PM B31.00006 Two-level systems and a low-energy oscillator: Excitation transfer and energy exchange, PETER HAGELSTEIN, IRFAN CHAUDHARY, Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, MA 02139 — We first consider one set of matched two-level systems that are coupled to an oscillator with an energy much lower than that of the two-level systems. We show that energy can be exchanged between the two systems coherently, illustrating the effect both with the results of a direct numerical calculation, and also with an analytic result. We then show that excitation can be transferred between two sets of two-level systems that are coupled indirectly through a low-energy oscillator. We illustrate the effect with a direct numerical calculation, and also with an analytic result. Finally, both of these effects are significantly enhanced when energetic loss channels are open to the oscillator. This is illustrated with numerical and analytic calculations.

12:27PM B31.00007 Material Science Developments Enhancing Excess of Power Reproducibility, V. VIOLANTE, M. BERTOLOTTI, E. CASTAGNA, M. MCKUBRE, F. SARTO, C. SIBILIA, F. TANZELLA, Z. ZILOV, ENEA Frascati Research Center, Frascati (Italy) — Material science research activities have been carried out in order to increase the reproducibility of the excess of power production during electrolytic loading of palladium with deuterium. In the past a wide work was developed to obtain a metallurgical structure of the palladium able to ensure a significant loading of deuterium above the threshold of 0.95 (D/Pd atomic fraction). It was observed that the high loading of the Pd cathode with deuterium was a necessary condition to have the occurrence of the excess of power production. The more recent work was mainly oriented to optimize the material properties in order to have a significant improvement of the reproducibility of the excess of power. During the last campaign of experiments more than 50% of the experienced cathodes produced excess of heat ranging from 30% up to more than 100% of the input.

1 La Sapienza University, Roma Italy
2 SRI International Menlo Park
3 Energetics Technology, Omer (Israel)

12:39PM B31.00008 Quantization of Differences Between Atomic and Nuclear Rest Masses and Self-organization of Atoms and Nuclei, F.A. GAREEV, I.E. ZHIDKOV, Joint Institute for Nuclear Research, Dubna, Russia — We come to the conclusion that all atomic models based on either the Newton equation and the Kepler laws, or the Maxwell equations, or the Schrodinger and Dirac equations are in reasonable agreement with experimental data. We can only suspect that these equations are grounded on the same fundamental principle(s) which is (are) not known or these equations can be transformed into each other. We propose a new mechanism of LENR: cooperative processes in the whole system nuclei + atoms + condensed matter - nuclear reactions in plasma - can occur at smaller threshold energies than the corresponding ones on free constituents. We were able to quantize[1] in quantum-mechanologically the first time the differences between atomic and nuclear rest masses by the formula: \(\delta M_{1/n_2} = n_1 n_2 \times 0.0076294 \text{ (MeV/))}^2\), \(n_1=1,2,3,...\). Note that this quantization rule is justified for atoms and nuclei with different A, N and Z and the nuclei and atoms represent a coherent synchronized systems - a complex of coupled oscillators (resonators). The cooperative resonance synchronization mechanisms can explain how electron volt (atomic-) scale processes can induce and control nuclear MeV (nuclear-) scale processes and reactions.


12:51PM B31.00009 Anomalous Nuclear Phenomena Associated with Ultrafast Processes, XINGLIU JIANG, XIAOPING ZHOU, LIJUN HAN, LIYIN WANG, Department of Physics, Beijing University of Aeronautics and Astronautics, Beijing, China, 100083 — Localized nuclear reactions on the tips of the surface of electrodes in electrolysis cells have been observed by using solid detectors CR-39 and autoradiography in our laboratory at the period of May, 1989. A physical model[2] of transient vortex dynamics with torsion coherence with the zero point energy has been proposed by Xingliu Jiang based on the ultrafast processes of triple phases area of tip effect on the electrode surface. Considering the large equivalent capacitance of electrochemical double layer, it is presumed that the double layer can exhibit nonlinear electrical response with spatial and temporal variations confined to microscopic areas by tip effect. Recent work[3] reveals that nuclear reactions which usually occur at the field of high energy states, could be created in the systems of far from equilibrium with nonlinear behavior at room temperature. Our current understanding of science is like a puzzle with a large missing piece-zero point energy.


1:03PM B31.00010 Search for Charged Particle Tracks Using CR-39 Detectors to Replicate the SPAWAR Pd/D External Field Co-Deposition Protocol, WINTHROP WILLIAMS, Department of Electrical Engineering and Computer Science, University of California at Berkeley, Berkeley, CA 94720 — A solution of 0.031 M PdCl2 and 0.30 M LiCl in D2O was electrolyzed between Pt anode and Ag cathode wires at currents ranging from 100 microamps to 100 milliamps in two similar series-connected plastic butyrate cells. Pd and D were co-deposited onto the Ag cathodes. CR-39 detectors adjacent to the Ag cathode wires were used to search for charged particle tracks in each cell. An external magnetic field was applied to one of the two cells. Throughout the experiment, ambient temperature, current through and voltage across each cell were monitored. Current was applied in a stepped fashion, starting at 0.1mA increasing by factors of 2 to 5 up to 100mA.

Monday, March 5, 2007 2:30PM - 5:30PM — Session D1 DCMP: Induced Superconductivity in Carbon Nanotubes and Graphene, Colorado Convention Center Four Seasons 2-3

2:30PM D1.00001 Induced Superconductivity in Nanowires and Nanotubes, LEO KOUVENHOVEN, Kavli Institute of NanoScience, TU Delft — We study experimentally electron transport in 1 dimensional semiconductor nanowires (consisting of InAs and InP combinations) and carbon nanotubes. The wires are connected to superconducting source-drain contacts with gate electrodes in the substrate or on the surface. In the regime of weak coupling to the contacts we observe Coulomb blockade effects. We present level spectroscopy including a determination of the spin states. In the regime of strong coupling to the contacts interference effects are observed. In this regime and using superconducting contacts, we find supercurrents flowing through InAs-nanowires over micrometer length scales. The critical current is tunable by gate voltage, thus realizing so-called Joffets[1]. When we define quantum dots in between superconducting contacts the direction of the supercurrent is determined by the single electron spin state in the quantum dot[2,3].

3:06PM D1.00002 Andreev reflection in graphene

3:42PM D1.00003 Superconducting Nanotube Dots

4:18PM D1.00004 Josephson junctions with tuneable single wall carbon nanotubes as barriers

4:54PM D1.00005 Gate-controlled superconductivity in diffusive multiwalled carbon nanotube

Monday, March 5, 2007 2:30PM - 5:30PM –
Session D7 DCMP: Signatures of Non-Abelian Quantum Hall States

2:30PM D7.00001 Non-Abelian quantum Hall states of fermions and bosons

The Smoluchowski Effect and Step-Edge Behavior of Nanocars and Azofullerenes, CHETAN NAYAK, UC Los Angeles — No abstract available.

Monday, March 5, 2007 2:30PM - 5:30PM — Session D27 DCMP: Fullerenes, Nano-membranes, and Quasicrystals Colorado Convention Center 301

2:30PM D27.00001 The equilibrium and electronic structure of large icosahedral fullerenes using an all-electron fully analytic density functional theory, RAJENDRA ZOPE, University of Texas at El Paso, BRETT DUNLAP, US Naval Research Laboratory — We have recently developed a fast, variational and fully analytic density functional theory (ADFT). Instead of numerical integration it employs analytic integration using Gaussian basis sets and the calculus of variations to express the molecular orbitals as well as the Kohn-Sham potential in linear-combination of atomic orbital form. We first parametrize the ADFT to provide the experimental geometry of C_{60} fullerene. Using this parametrization, the triple zeta 6-311G(d,p) orbital basis, and density fitting with exchange-correlation bases that include up to f functions, the geometries of C_{2160}, C_{540}, C_{960}, and C_{2160} fullerenes are optimized. The equilibrium structures of these fullerenes are polyhedral in nature, confirming the previous predictions by tight-binding methods. Bond distances are converging towards those of graphene. The evolution of electron removal energies, electron affinities, and singlet excitation energies from C_{60} to C_{2160} is studied using the ΔSCF and transition-state methods.

1 Also at, Department of Electrical and Computer Engineering, Howard University, Washington DC

2:54PM D27.00003 The Smoluchowski Effect and Step-Edge Behavior of Nanocars and Azofullerenes, ANDREW OSGOOD, YASUHIRO SHIRAI, TAKASHI SASAKI, J.M. TOUR, K.F. KELLY, ELECTRICAL AND COMPUTER ENGINEERING DEPARTMENT, RICE UNIVERSITY COLLABORATION — The nanocar molecule - four fullerene wheels connected by rotating alkyne axles to a central chassis - was the first molecule designed and fabricated specifically for nanoscale manipulation. We have investigated the imaging and manipulation of the nanocar molecule on Au(111) by variable-temperature STM, with specific focus on their unique dynamic step-crossing and -straddling abilities. Our static analysis of the molecules adsorbed at step edges under the influence of the Smoluchowski effect has begun to explain the complex interactions of their behavior in these regions, with an eye towards surface manipulation in three dimensions. Further manipulation studies also attempt to elucidate the fullerene-substrate interactions that make rolling manipulation possible, with special attention paid to the azofullerene dimer - one of the first specifically designed and tested molecules incorporating two simple mechanical functions – actuation of the “azo” unit and rolling/rotation of the wheel-like fullerenes.
3:06PM D27.00004 Cage-Core Interactions in Fullerenes Enclosing Metal Clusters with Multiple Scandium and Yttrium Atoms. LIU DAN, FRANK HAGELBERG, Jackson State University — Pronounced stability has been reported for metallofullerenes of the form NSCN1CN (N = 68, 78) /1/. In response to these and related findings, Density Functional Theory studies have been performed on the relation between cage-core interactions and the geometry as well as stability of endofullerenes with metal impurities containing Sc and Y. Substantial electron transfer from the metal core to the fullerene cage combines with electron backdonation, involving the interaction between the occupied orbitals of the negatively charged cage and the unoccupied d orbitals of the positively charged core. The initial 4n + 2 rule, well established in organic chemistry, is shown to provide a valuable heuristic tool for understanding the intramolecular electron transfer and the related stability gain /1/. The usefulness of the aromaticity concept for explaining and predicting the architecture of metallofullerenes is further exemplified by the units Sc2C8B4 and Y2C8B4 which were analyzed in spin triplet and singlet conditions. The Sc2 core turns out to be realized by two separated ions, while Y2 forms a bound subunit. These findings are in agreement with conclusions based on the 4n – 2 rule, assisted by Nucleus Independent Chemical Shift (NICS) calculations /1/. Stevenson, S.; Fowler, P.W.; Heine, T.; Duchamp, J.C.; Rice, G.; Glass, T.; Harich, K.; Hadju, F.; Bible, R.; Dorn, H.C. Nature, 2000, 408, 427, /2/ S. S. Park, D. Liu, F. Hagelberg, 1

3:18PM D27.00005 Hydrogen Storage in Novel Carbon-based Nanostructured Materials. ERIN WHITNEY, CALVIN CURTIS, CHAIWAT ENGRATKUL, MARK DAVIS, KIM JONES, PHILIP PARILLA, LIN SIMPSON, ANNE DILLON, NREL, NREL TEAM — One of the biggest challenges facing a future hydrogen economy is that of onboard vehicular hydrogen storage, for which novel carbon-based nanostructured materials have emerged as potential candidates. Towards this end, we present the synthesis and characterization of “bucky dumbbell”, a new organometallic compound comprised of two buckyballs complexed to a central iron atom. This new compound has been characterized using both 13C solid-state NMR and Raman spectroscopy, and electron spin paramagnetic resonance spectroscopy reveals the presence of Fe3+. Temperature-programmed desorption has revealed a new hydrogen binding site via the appearance of a peak centered at approximately -50 °C, indicating the hydrogen is stabilized at a temperature significantly above that expected for physisorption but still lower than that of C-H bond formation. Comparison with C60 under the same hydrogen exposure and heating conditions shows almost no hydrogen adsorption, and the exact binding energy (or desorption activation energy, E_A) for the bucky dumbbell shows an enhanced value of ~6.2 kJ/mol. Initial volumetric analyses conducted at 77K and 3 bar show a storage capacity of ~0.4 wt%. The synthesis and analysis of other novel fullerene-based organometallic hydrogen complexes will also be discussed.

3:30PM D27.00006 Microscopic ESR study of N@C60 using a Magnetic Resonance Force Microscope. P. BANERJEE, D. V. PELEKHOV, K. C. FONG, I. H. LEE, P. C. HAMMEIL, Dept. of Physics, Ohio State University, Columbus OH 43210, W. HARNEIT, Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — We report electron spin resonance studies of the endohedral fullerene N@C60 using the novel technique of magnetic resonance force microscopy (MRFM). These studies are performed at temperatures down to 1 K on both thin films of N@C60 and in samples where the endohedral fullerene is incorporated into a bulk crystalline matrix. Utilizing the large magnetic field gradients (~ 10^5 Tesla/meter) in the vicinity of our micromagnetic probe tip, we are able to selectively probe the electron spins in sub-micron volumes. Further, our schemes for spin manipulation allow us to measure the spin-lattice relaxation rate (T1^-1) with a spatial resolution in one dimension of approximately 20 nanometers. We will also discuss our efforts to improve the sensitivity of our microscope for detecting individual electronic spins.

3:42PM D27.00007 Dimensional evolution of the electronic and structural properties of K3C60 multilayers studied by Scanning Tunneling Microscopy. YAYU WANG, RYAN YAMACHIKA, ANDRE WACHOWIAK, MIKE GROBIS, MIKE CROMMIE, Department of Physics, University of California at Berkeley — We investigate the effect of dimensionality on the properties of potassium doped C60 (K3C60) by studying thin films with precisely controlled doping levels and layer structures using scanning tunneling microscopy and spectroscopy. We observe systematic variation in spatial and electronic structure as the films change from the 2D to the quasi-3D regime. In metallic K3C60, the large electronic density of states at the Fermi level (E_F) is seen to split, with a small gap opening at E_F. In the Jahn-Teller-induced K3C60 insulator, the energy gap around E_F increases monotonically with increased film thickness. In K3C60, the spectra change from a re-entrant metal to an insulator in the third layer. These trends can be explained considering the increase of Coulomb repulsion in multilayers as screening from the metal substrate is reduced. These results highlight the role of strong electron correlation and dimensionality in determining the properties of doped fullerides.

3:54PM D27.00008 Crystal structure of Rb4C60 under pressure1. ASHFIA HUQ, Oak Ridge National Laboratory, PETER W. STEPHENS, Stony Brook University — We show that Rb4C60 transforms from its orientationally disordered tetragonal structure at ambient pressure to an orthorhombic phase in the neighborhood of 0.4 GPa. Lattice parameters, interfullerene distances, and closest Rb-C distances evolve continuously up to 2.2 GPa. Rietveld refinements establish that the high pressure phase is isostructural to Cs4C60. Detailed results on the moleculardynamics and the other properties for C60, C70 and C61H23-nanowhiskers(NWs) by x-ray diffraction and solid state NMR. The previous observed conducting phase at 0.8 GPa is therefore structurally distinct from the ambient pressure insulator.

4:06PM D27.00009 Structural characterization and molecular dynamics of fullerene or fullerene-derivative nanowhiskers. HIRONORI OGATA, SATORU MOTOHASHI, Hosei University — Recently, a new type of fibrous fullerene crystals called fullerene nanowhisker has been reported by a liquid-liquid interfacial precipitation method using saturated m-xylene solution of fullerene and isopropl alcohol. Considerable interests have been generated in the structure and properties of fullerene or fullerene-derivative nanowhiskers. In this study, we present the results of structural characterization and molecular dynamics of C60, C70 and C61H23-nanowhiskers(NWs) by x-ray diffraction and solid state NMR. The XRD pattern of as-grown C60-NWs have a hexagonal structure with lattice constants of a=33.72 and c=10.126. Both solid-state 13C-CP/MAS and wideline

1Work at the NSLS and APS was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contracts DE-AC02-98CH10886 and W-31-109-Eng-38.

13C-NMR measurement clearly shows that m-xylene molecules are included in NWs. Both lineshape and spin-lattice relaxation time of wideline 13C-NMR measurements clearly show that C60-NWs exhibit the depressed transition at 250 K. Detailed results on the molecular dynamics and the other properties for C60, C70 or C61H23-NWs will be presented.
4:18PM D27.00010 Formation of SiC Clusters with Bucky Diamond Structures1, M. YU, C. GHOSH, C.S. JAYANTHI, S.Y. WU, University of Louisville — SiC clusters with bucky diamond structures have been found in a quantum-mechanical molecular dynamics study based on our recently developed self-consistent and environment dependent Hamiltonian in the framework of a linear combination of atomic orbitals [1]. Starting from a spherically truncated bulk diamond structure, stable structures of SiC clusters containing 147 atoms were studied for various compositions of Si and C atoms. In particular, the following initial configurations were considered: (i) C-rich configuration with Si-core, (ii) Si-rich configuration with C-core, and (iii) an almost equal admixture Si and C atoms. It is found that in the first case Si atoms are dragged to the exterior and a cage-like structure formed, while in the second case some C atoms remain in the interior region and some move to the exterior region forming distorted tetrahedral structures with Si atoms. Finally, in the third case, the bucky-diamond structure is obtained, where the interior has a diamond-like structure and the exterior a fullerene-like structure. The reason why (Si)C147 clusters form different stable structures can be understood based on hybridization characteristics of Si (sp3) and C atoms (sp1, sp2, and sp3), respectively. [1] Leahy et al. Phys. Rev. B74, 155408 (2006).

1 Sources of funding: KSEF and DoE/EPSCoR.

4:30PM D27.00011 In-situ microscopic investigations of the nucleation and growth of C60 films on Bi(0001)/Si(111) . JERZY T. SADOWSKI, T. NISHIHARA, A. AL-MAHBOOB, Y. FUJIKAWA, K. NAKAJIMA, T. SAKURAI, Institute for Materials Research, Tohoku University, Sendai, Japan, T. NAGOI, National Institute for Materials Science, Tsukuba, Japan — Growth of epitaxial C60 films on Si is of particular interest for technological reasons. However, strong interaction between the C60 molecules and the clean Si induces film growth in the Stransky-Krastanov mode with only local ordering in the first monolayer. Passivation of the Si dangling bonds — for example with hydrogen — leads to van der Waals bonding of adsorbates and thus higher degree of crystallinity in C60 film, but the true relation between surface properties, and the crystallinity of the fullerene film is not yet fully understood. In this work, C60 thin films were grown by UHV deposition on Si(111) substrate covered with thin Bi(0001) passivation layer. Real-time, dark-field low-energy electron microscopy (LEEM) investigation of the growth revealed that C60 film nucleates in fcc(111) phase, having an epitaxial relation with the Bi(0001) surface. At a growth temperature of ~400K, preferential nucleation of C60 at Bi twin boundaries has been detected. Low-energy electron diffraction (LEED) confirmed that film had a single orientation and an excellent crystallinity. The in-plane lattice parameter in the C60 films with thickness up to 3ML has been measured to be 10.04 ± 0.02 Å, which is very close to the bulk value of 10.01 Å.

4:42PM D27.00012 Elastic strain-sharing as a means of fabricating strained-Si(110) nanomembranes1, SHELLEY SCOTT, ARRIELLE OPOTOWSKY, DONALD SAVAGE, MICHELLE ROBERTS, MAX LAGALLY, University of Wisconsin-Madison — Hole mobility is higher in Si(110) than it is in Si(001), and straining Si(110) produces further improvements, making strained-Si(110) desirable for p-MOS devices. We describe elastic strain sharing in Si:SiGe:Si(110) heterostructure membranes, which generates flexible, transferable, and dislocation-free strained-Si(110) nanomembranes. Membranes are grown by chemical vapor deposition on the Si template layer of (110) silicon-on-insulator (SOI) substrates. Selective etching of the buried oxide layer `releases' the epitaxial tri-layer system. X-Ray diffraction measurements show that the heterostructure elastically relaxes by transferring strain from compression in the alloy layer, into tensile strain in the Si layers, and we will discuss the achieved mobility values. The XRD line scans exhibit narrow peak widths and thickness fringes, which are both signatures of high-quality (negligible dislocation density) single-crystal strained-Si.

1 Research supported by NZ Foundation for Research Science & Technology, DOE, and NSF-SURE Program

4:54PM D27.00013 Dislocation-free, uniformly strained Si fabricated by Si nano-membrane (SiNM) technology1, CHANAN EUARUSKAKUL, ZHIWEI LI, DONALD E. SAVAGE, MAX G. LAGALLY — It is known that the interface of a thin film with the substrate on which it is grown plays an important role in dislocation nucleation and kinetic critical thickness. A crystalline-amorphous interface reduces the line energy of dislocations and makes strained structures on SiO2 [e.g., strained-Si-on-insulator (sSOI)] or a strained SiGe film grown on SOI, susceptible to dislocation formation. We describe fabrication of elastic strain-sharing Si nanomembranes and demonstrate that these strained structures are more thermally stable than strained structures on noncompliant substrates. Our studies with low-energy electron microscopy (LEEM) and x-ray absorption spectroscopy (XAS) show that the structures have a more uniform strain than the strained Si fabricated by conventional SmartCut® sSOI technology.

1 Research supported by DOE, NSF and AFOSR

5:06PM D27.00014 Mechanism of quasicrystal nucleation and growth. SHARON GLOTZER, AARON KEYS, Department of Chemical Engineering, University of Michigan — On cooling, liquids ordinarily solidify into glasses or into crystalline phases with long- range periodic ordering. However, it is also possible to form quasicrystals, ordered solids with long-range aperiodicity. Although quasicrystals have been observed in many materials, their formation is poorly understood. We present the results of a molecular simulation study to elucidate the process by which quasicrystals form from supercooled liquids. We show that, as has been speculated in previous theoretical and experimental works, icosahedral clusters play a significant role in quasicrystal formation. Specifically, icosahedral clusters facilitate the formation of the so-called quasicrystal “critical” nucleus, and, together with phasons, facilitate the complicated mechanism that allows quasicrystals to grow aperiodic structures via local interactions. Our findings suggest that direct correlations between liquid ordering and solid structure may be a requisite property for quasicrystal-forming systems, and is consistent with the class of systems that are known to form quasicrystals experimentally.

5:18PM D27.00015 Specific heat of rhombohedral C60 polymer in the temperature range of 2-300K1, MIN GU, GUANGLIEI CUI, LIHANG WANG, XIAO CHEN, National Laboratory of Solid State Microstructures, Nanjing University — Under high temperature of 700 K and high pressure of 6 GPa, we have prepared a batch of C60 polymer. XRD data confirmed it is rhombohedral phase and solid 13C NMR showed a formation of sp3 bond between two neighbor C60 in (111) plane. We have measured the specific heat of C60 polymer and pristine C60 by PPMS in the range some C atoms and 300 K. Temperature dependence result of pristine C60 agreed well with previous report. For C60 polymer, above T~30 K it is found that temperature dependence of the specific heat is similar to that of pristine C60 besides an anomaly from order-disorder phase transition at 260K, but in range from 2 to 80K the specific heat is much less than that of pristine C60. Assuming three- (3D) and two-dimensional (2D) Debye phonon modes to contribute respectively to the specific heat in different temperature zone, the calculated values of specific heat have got a good agreement with the experimental data in the whole temperature range. These results show the 2D planar modes but not 3D modes are a dominator to the specific heat of C60 polymer, and the low-frequency intermolecular modes of C60 lattice are restrained in the case of C60 polymer by sp3 bonds from 2 to 2 cycleaddition reaction.

1 This work was supported by grants from the MOST 973 Program of China (No. 2006CB705600), the NSF of China (No. 10674060) and the Jiangsu Province Foundation of Natural Science (No. BK2006109).

and thermal conductivities as well as tremendous mechanical strength. Here we report a new technique to measure the thermal properties of nanosystems. We as low as 2400K. Carbon nanotubes (also sp-2) capitalize on the extraordinary strength of the sp-2 hybridized carbon-carbon bond and exhibit high electrical conductivity but is meta-stable and transitions to graphite at elevated temperatures. Graphite (sp-2) is electrically conducting but sublimes at temperatures bonding creates a wealth of extraordinary physical properties. Of the two common allotropes of carbon, diamond (sp-3 bonded) exhibits record thermal BRIAN M. KESSLER, THOMAS D. YUZVINSKY, HENRY GARCIA, ALEX ZETTL, University of California, Berkeley — The versatility of carbon-carbon

2:42PM D31.00002 Characterization and Reduction of 1/f Noise in Carbon Nanotube Devices
YU-MING LIN, PHAEDON AVOURIS, IBM T. J. Watson Research Center — 1/f noise is a ubiquitous fluctuation in semiconductors and metals. Unlike other types of fluctuations such as the thermal noise and the shot noise, 1/f noise increases with decreasing device dimension and is highly dependent on the material quality and interface properties. Therefore, the noise characteristics in nanoscale devices are usually dominated by the 1/f-type fluctuations. Here we perform a systematic study on the 1/f noise of carbon nanotube devices consisting of individual single-wall carbon nanotubes. We have examined the impact of the contact and the substrate to the 1/f noise in carbon nanotube devices in order to reduce the 1/f noise level. By eliminating the charge traps associated with oxide substrates, we found that the 1/f noise in carbon nanotube devices can be lowered by up to two orders of magnitude. These results reveal important factors contributing to the 1/f noise source in carbon nanotube devices, and are of great importance for applications based on carbon nanotubes.

2:54PM D31.00003 Tunneling spectroscopy in carbon nanotubes
YUNG-FU CHEN, Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign, GASSEME AL-ZOUBI, NORMAN BIRGE, Department of Physics and Astronomy, Michigan State University, NADYA MASON, Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign — Carbon nanotubes are one-dimensional metallic or semiconducting wires that serve as good model systems to study Luttinger liquids, in which electron-electron interaction are essential to electronic transport. Luttinger behavior has previously been measured via transport through the ends of nanotubes. We have fabricated novel nanotube devices with three-terminal configurations—two normal contacts at the ends and one non-invasive superconducting tunnel probe in the middle. This configuration is well-suited to tunnel spectroscopy studies of bias-dependence, non-equilibrium effects, and carrier interactions in nanotubes. We present results on low-temperature tunneling measurements performed using this configuration.

3:06PM D31.00004 ABSTRACT WITHDRAWN

3:18PM D31.00005 Experimental and Theoretical studies on Synthesis of Massively Aligned Single-Walled Carbon Nanotubes and Transistor Applications
KOUNGMIN RYU, CHONGWU ZHOU, Univ. of Southern California — Synthesis of highly aligned single-walled carbon nanotubes with controlled diameters is an important step towards manufacturable ultra dense carbon nanotube integrated circuits. We have successfully demonstrated the synthesis of highly aligned carbon nanotube arrays on a-plane sapphire and miscut quartz substrates. Our calculation of the Lennard-Jones potential clearly reveals that a nanotube would lie normal to the c-axis of a-plane sapphire for minimized potential energy, consistent with our experimental observation. In addition, we have developed a patterned growth method to control both the orientation and position of the aligned nanotubes. This was achieved by using photolithography to deposit catalyst at desired locations on sapphire or quartz, followed by CVD growth of the aligned nanotubes. Furthermore, based on aligned nanotubes array, we have fabricated transistors combined with Pd source/drain contact and HfO2 high-k dielectric material. The transistors show on/off ratios up to 1000000 and subthreshold swings down to around 150 mV/decade. Our aligned Nanotube growth work paves the way for a better understanding of the aligned synthesis and could eventually lead to the growth of aligned nanotubes with controlled diameters and even chiralities. Moreover, transistors approach based on massively aligned Nanotube arrays may work as a platform for explorations of nanotube integrated circuits.

3:30PM D31.00006 Extreme Thermal Stability of Carbon Nanotubes
GAVI BEGTRUP, KEITH G. RAY, BRIAN M. KESSLER, THOMAS D. YUZVINSKY, HENRY GARCIA, ALEX ZETTL, University of California, Berkeley — The versatility of carbon-carbon bonding creates a wealth of extraordinary physical properties. Of the two common allotropes of carbon, diamond (sp-3 bonded) exhibits record thermal conductivity but is meta-stable and transitions to graphite at elevated temperatures. Graphite (sp-2) is electrically conducting but sublimes at temperatures as low as 2400K. Carbon nanotubes (also sp-2) capitalize on the extraordinary strength of the sp-2 hybridized carbon-carbon bond and exhibit high electrical and thermal conductivities as well as tremendous mechanical strength. Here we report a new technique to measure the thermal properties of nanosystems. We apply this technique to determine the extreme high temperature stability and thermal conductivity of multiwalled carbon nanotubes.

3:42PM D31.00007 High Current All-Semiconductor Carbon Nanotube Electronics
GUANGYU ZHANG, PENGFEI QI, XINRAN WANG, YUERUI LU, XIAOLIN LI, RYAN TU, SARUNYA BANGSARUNTIP, DAVID MANN, LI ZHANG, HONGJIE DAI, Department of Chemistry, Stanford University, Stanford, CA 94305 — Existence of both metallic and semiconducting carbon nanotubes in as-grown materials has hindered the development of nanotube electronics. A gas-phase plasma hydrocarbonation reaction is shown here to selectively etch and gasify metallic nanotubes, retain semiconducting nanotubes in near-pristine forms without covalent modification, and narrow down diameter distribution of the semiconductors. 100% of purely semiconducting nanotubes are obtained and connected in parallel for high-current transistors without shorts by metallic species. The 'dry' chemical approach is scalable and compatible with existing semiconductor processing technology for future integrated circuits.

*We thank Intel and MARCO MSD for support.*

3:54PM D31.00008 Chemoresistance of carbon nanotube circuits incorporating electrochemically-decorated defects
VAIKUNTH KHALAP, ALEXANDER KANE, PHILLIP COLLINS, University of California, Irvine — The chemical functionalization of single-walled carbon nanotubes (SWNTs) is of broad interest, since it allows SWNT properties to be widely tailored. We specifically investigate SWNT devices with single point functionalizations. Standard fabrication techniques are supplemented by an electrochemical point-oxidation process that creates insulating defects into otherwise pristine SWNTs. Selective electrochemistry subsequently deposits metal onto the insulating site(s) and restores the device conductivity. Furthermore, the resulting circuits inherit the chemical sensitivity of the metal deposits. For example, nickel deposits produce an air-sensitive reconnection which readily oxidizes in air back to an open circuit. Palladium deposits are air stable but highly sensitive to hydrogen gas. The interaction of Pd with point defects appears to entirely reproduce the reported characteristics of SWNT-based hydrogen sensors.
4:06PM D31.00009 Electron channeling through an individual multiwall carbon nanotube .
GUANGYU CHAI, Department of Physics, University of Central Florida, Orlando, FL 32816, USA, HELGE HEINRICH, LEE CHOW, Department of Physics, Advanced Materials Processing and Analysis Center, University of Central Florida, Orlando, FL 32816, USA, THOMAS SCHENKEL, E. O. Lawrence Berkeley National Laboratory, Berkeley, Ca 94720, USA — The hollow structure of the carbon nanotube (CNT) provides a significant chance to use it for the channeling of charged particles and associated channeling radiation. However, the nano size of the CNTs makes them difficult to precisely control the position and the orientation. We successfully prepared a monolithic multiwall CNT with a graphic shield by chemical vapor deposition technique. The graphic shield provides a handle which allows the manipulation of the supported CNTs. A single CNT collimator is fabricated with focused ion beam technique. The channeling through the single CNT collimator is demonstrated for the first time.

4:18PM D31.00010 Test for superconductivity in individual end-bonded MWNTs .
Y. SUN, S. CHEN, J.Y. HUANG, Z.F. REN, J.I. OH, M.J. NAUGHTON, M. VAZIRI, U. Mich.-Flint — Takesue et al. [1] recently reported 12K superconductivity in templated arrays of ~ 10^4 "end-bonded" multi-walled carbon nanotubes (MWNTs). They attributed the occurrence of superconductivity to intershell (interlayer) effects within each MWNT. We have tested this by preparing and measuring individual end-bonded MWNTs, which were grown by arc-discharge without catalyst. High resolution TEM showed they had typical outer (inner) diameters of 10 - 15 nm (1-2 nm), with no visible defects, values verified by AFM and electrical measurements. We also verified by TEM that, as grown, the nanotube ends were closed. We then used a novel nanolithographic approach to facilitate end-bonding (i.e. contacting all layers), which was subsequently verified in I - V tests. Four-probe resistivity was measured for several such individual end-bonded MWNTs, to 1.4 K, including the use of current densities smaller than those used in Ref. 1. No evidence for superconductivity was found.

5:06PM D31.00014 Torsional Electromechanics of Carbon Nanotubes .
ERNESTO JOSELEVICH, TZAHII COHEN-KARNI, LIOR SEGEV, ONIT SRUR-LAVI, SIDNEY R. COHEN, Weizmann Institute of Science, Israel — Carbon nanotubes are known to be distinctly metallic or semiconducting depending on their diameter and chirality. Here we show that continuously varying the chirality by mechanical torsion can induce conduction oscillations, which can be attributed to metal-semiconductor periodic transitions. The phenomenon is observed in multi-walled carbon nanotubes, where both the torque and the current are shown to be carried predominantly by the outermost wall. The oscillation period with torsion is consistent with the theoretical shifting of the corners of the first Brillouin zone of graphene across different subbands allowed in the nanotube. Beyond a critical torsion, the conductance irreversibly drops due to torsional failure, allowing us to determine the torsional strength of carbon nanotubes. Our experiments indicate the production of a non-equilibrium population of RBM phonons analogous to the non-equilibrium optical and zone-boundary phonon population observed previously to limit transport in substrate-supported and suspended nanotube devices [1-3]. Finally, we are also conducting simultaneous Raman spectroscopy and electrical measurements on our devices to study the signatures of electron-phonon scattering in Raman data. We will report our latest findings in this regard. 1. Z Yao et al, Phys Rev Lett 84, 2941 (2000) 2. E Pop et al, Phys Rev Lett 95, 195505 (2005) 3. M Lazzeri et al, Phys Rev Lett, 95, 236802 (2005)

5:18PM D31.00015 Effects of Torsional Strain in Single Wall Carbon Nanotubes.
HYUNGBIN SON, Massachusetts Institute of Technology, XIAOJIE DUAN, YINGYING ZHANG, Peking University, GEORGII SAMSONIDZE, MILDRED DRESSELHAUS, JING KONG, Massachusetts Institute of Technology, JIN ZHANG, Peking University — Since it was predicted that the electronic properties of single wall carbon nanotubes (SWNTs) can be tuned drastically by strain, strain in SWNTs was intensively studied. Particularly, the effects of uniaxial strain on electronic and vibrational properties of SWNTs have been reported in several experimental works. However, little experimental work has been reported on other types of strain such as torsional strain. Our previous work has reported that we can induce torsional strain in SWNTs using AFM manipulation and that torsional strain has distinctive signature in various vibrational modes. In this work, we further investigate the effect of torsional strain on the vibrational modes of SWNTs in detail: frequency shift on different symmetry modes, mode splitting due to symmetry breaking, and changes in electron-phonon matrix elements.

This work was supported by NSFC (20573092, 20673004, and 50521001) and FOKYING TUNG Education Foundation (94012). H. Son and J. Kong acknowledge support from the Intel Higher Education Program. M.S. Dresselhaus acknowledges support from NSF DMR 04-05538.
2:42PM D41.00002 Spin-polarized metastable-atom deexcitation spectroscopy study of Xenon-adsorbed iron surfaces , YASUSHI YAMAUCHI, National Institute for Materials Science, MITSUNORI KURAHASHI, TAKU SUZUKI, PRESTO, Japan Science and Technology Agency, XIA SUN, ZHONGPING WANG — The electron spin polarization at the interface between nonmagnetic and ferromagnetic environments is one of the essential factors that may alter the spin transport phenomena. To investigate fundamental aspects of induced spin polarization we have examined the adsorbate-covered magnetic surfaces by means of spin polarized metastable-atom deexcitation spectroscopy (SPMDS). Use of spin-polarized metastable helium atoms in triplet states moving at thermal energies gives rise to the ultimate surface sensitivity. Although Xenon can adsorb on surfaces at low temperatures by the van der Waals force, no electron exchange with surfaces, especially no spin interaction, is expected because of its closed shell structure. XPS spectra measured for Xenon-adsorbed iron surfaces show three prominent peaks that are the same as those previously reported for other surfaces by D. M. Oro, et al. [Phys. Rev. A 49 (1994) 4703]. Two peaks \( (2P_{3/2}, 2P_{1/2}) \) at higher kinetic energies exhibit clear spin asymmetries while the other low energy peak has no appreciable spin asymmetry. The spin asymmetries will be discussed on the basis of spin polarization and deexcitation processes of metastable atoms.

2:54PM D41.00003 Homochiral magnetism in low-dimensional magnets , STEFAN BLUGEL, MARCUS HEIDE, GUSTAV BHIHLAYER, IFF, Forschungszentrum Juelich, 52425 Juelich, Germany, IFF-1 TEAM — Spin structures observed in nanomagnets are commonly explained on the basis of the Heisenberg exchange and the magnetic anisotropy. Electrons propagating in the vicinity of inversion-asymmetric environments such as of surfaces, interfaces or in ultrathin films can give rise to the Dzyaloshinskii-Moriya (DM) interaction, typically unimportant for metals. Surprisingly, there is no hard number known from theory about its strength, as this requires supercomputing at the cutting edge. One deals with long-ranged complex magnetic structures in low-dimensions. Since the DM interaction arises from spin-orbit coupling, each atom of the long range structure has a different electronic environment and previous strategies, e.g. applying the generalized Bloch theorem, fail. But if DM is important, the so-far anticipated collinear magnetism become unstable, and homochiral spin structures occur. We developed a perturbative strategy implemented into the FLAPW code FLEUR which can cope with this challenge. We show by first-principles calculations based on the vector-spin density formulation of the DFT that the DM interaction is indeed sufficiently strong to compete with the interactions that favor collinear spin alignment. We predict new magnetic phases in thin films which had been overlooked during the past 20 years.

3:06PM D41.00004 Temperature-induced Domain Shrinking in Dipolar Frustrated Ising Ferromagnet , DANIELO PESCA, ALESSANDRO VINDIGNI, OLIVER PORTMANN, Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland, PAOLO POLITI, Istituto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche, 50019 Sesto Fiorentino, Italy — Motivated by recent experimental observations on ultrathin Fe/Cu(001) films, we performed a theoretical analysis of magnetic domain pattern evolution in 2D Dipolar Frustrated Ising Ferromagnet. Due to the competition between long-ranged dipolar interaction and nearest neighbor ferromagnetic exchange interaction, the ground state is given by a succession of saturated domains of positive and negative magnetization, which alternate in a sharp striped pattern of characteristic domain width \( L_\text{gs} \). Close to the Curie temperature \( T_c \), the Mean Field theory predicts the occurrence of a cosine modulation with a much smaller spatial period \( (L(T_c)) \). We found that these two limits are connected continuously in the temperature range \( 0 \leq T \leq T_c \). But, as translational invariance does not hold, the interplay between thermal fluctuations and the two competing interactions gives rise to a non-trivial magnetization profile at intermediate temperatures.

3:18PM D41.00005 Controlling Spin-Density Wave Periodicity in Thin Cr\(_{1-x}\)V\(_x\) Films , OLEG KRPIN, University of Oregon, ELI ROTENBERG, Advanced Light Source, S. D. KEVAN, University of Oregon — Chromium is an itinerant antiferromagnet with a spin-density wave (SDW) ground state driven by a nesting of Fermi surface sheets around the Gamma and H points of the Brillouin zone. Periodicity of the SDW plays an important role in mediating magnetic interactions in magnetic multilayer structures providing a giant magnetoresistance effect and potentially interesting for application in spintronic devices. Therefore control of SDW in thin chromium films is of the high importance. It requires a detailed understanding of phenomena related to stabilization of SDW. We used angle-resolved photoemission to characterize spin-density wave and Fermi surface topology in thin Cr\(_{1-x}\)V\(_x\) films as a function of the film thickness, temperature, composition and hydrogen surface coverage. A key feature of our results is the ability to control the magnetic structure of thin films of Cr with an external perturbation: balancing the surface energetic interactions favored commensurare state of SDW vs. the energy associated with Fermi surface topology stabilizing SDW incommensurate phase in the bulk.

3:30PM D41.00006 Manipulating spins using spin-valves of self-assembled molecular wires , VLADIMIR BURTMAN, VALY Z. VARDENY, University of Utah — We studied spin transport using spin-valves of self-assembled monolayer (SAM) devices sandwiched between two ferromagnetic electrodes, namely La\(_0.33\)Sr\(_{0.66}\)MnO\(_3\) (LSMO) and Co having different coercive fields. The SAM film contained isolated molecular wires that bond with both electrodes, in an otherwise insulating molecular matrix that bond only with one electrode. The relative resistance change, or magnetoresistance (MR), DR/R between the device resistance with the electrodes magnetizations parallel and anti-parallel to each other serves as a figure of merit and show spin injection through the isolated molecular wires. We found a giant MR of up to 80% at 10K. The MR response was measured at various temperatures and biasing voltages to obtain the complete magneto-transport characteristic properties of the organic spin-valve devices.

3:42PM D41.00007 ABSTRACT WITHDRAWN —
3:54PM D41.00008 Structural and magnetic properties of ferromagnetic metal-oxide films grown by polymer assisted deposition. M. JAIN, P. SHUKLA, M. F. HUNDLEY, A. K. BURRELL, T. M. MCCLESKEY, Q. X. JIA, Los Alamos National Lab — Ferromagnetic metal-oxide films such as doped lanthanum manganites have been extensively investigated over the past decade due to their potential applications in different fields. To grow these oxide films, the most widely used approaches are physical vapor deposition, chemical vapor deposition, and chemical solution deposition techniques. One of the challenges in solution-based processes of such oxide films has been to produce high quality multilayer films and at the same time to control the stoichiometry. We describe a solution route called polymer-assisted deposition (PAD) to grow such oxide films. High quality epitaxial single layer and multilayer coated films of Lao.67Sr0.33MnO3 (LSMO) and La0.67Ca0.33MnO3 (LCMO) have been grown by PAD. Multilayer is used to effectively take the advantages of both LSMO and LCMO with an aim to achieve large values of magnetoresistance (MR) near room temperature. An MR value as high as ~66% at 5 T has been obtained at 295K for the multilayer-coated films with LSMO/LCMO volume ratio of 60/40. The successful growth of epitaxial doped lanthanum manganites with desired properties by PAD shows that PAD is a feasible alternative approach to the growth of high quality metal-oxide films.

4:06PM D41.00009 Growth, structure and magnetic properties study of CVD cobalt layers1. NIRMALENDU DEO, HAROLD S. GAMBLE, The Queens University of Belfast, UK — Chemical vapour deposition (CVD) of cobalt was performed on oxidised silicon wafers at the temperature ranges 300-450°C, and found to be highly resistive (~250 kΩcm). As the deposition temperature increases the layer resistivity decreases and at 450°C the layer resistivity was reduced to ~100 kΩcm. Thus reduced resistivity is taken as evidence that the cobalt layer is purer. X-ray diffraction of the cobalt layers reveal both hcp and fcc peaks. The AES analysis shows that cobalt layer deposited at 300°C contains 26at% O, 10at% N. At higher deposition temperature of 400°C and above the impurities was 1% or less as documented by AES. At 300°C deposited cobalt layer the surface looks agglomerated as seen by SEM. At 350°C the grain structure is elongated and at 400°C and above the grain structure changes to hexagonal structure. At this temperature the cobalt phase-change occurs from hcp to fcc. The roughness of cobalt layer is higher in lower deposition temperature but this is only due to higher layer thickness measured by AFM. VSM shows, the saturation of magnetisation (M) for layers deposited at 400°C and 450°C is consistent with the bulk value of 1422 emu/cm3. As the cobalt deposition temperature increases the layer coercivity decreases from 705 to 400-Oe.

1This work was supported by Seagate Technology, Londonderry, UK

4:18PM D41.00010 Combinatorial Exploration of Magnetostriiction of Fe1-x-yGa0.5Mn0.5 Ternary Alloys1. JASON HATTRICK-SIMPERS, KYU SUNG JANG, University of Maryland, SAMUEL E. LOFLAND, Rowan University, NOBLE WOO, BRUCE VAN DOVER, Cornell University, MANFRED WUTTIG, ICHIRO TAKEUCHI, University of Maryland — Accurate heats of formation are necessary to examine phase stability and to aid in the modeling of phase transitions. However, most reported heats of formation of the ordered intermetallic phases, namely L10 Fe3Ga2 and Fe3Ga2, are several orders of magnitude smaller than observed. The composition spread samples were synthesized in an ultra high vacuum (10^-9 Torr) co-sputtering chamber. Magnetic properties were mapped through the use of a room temperature scanning SQUID and a high throughput magneto optical Kerr effect (MOKE) system. Magnetostriuctive measurements were performed on micromachined cantilever libraries at room temperature. The correlation between magnetic and magnetostrictive properties across the composition phase diagram of the two systems will be discussed.

1This work was supported by ONR-MURI-N000140610530

4:30PM D41.00011 Memory interference in stage-2 CoCl2 graphite intercalation. MASATSUGU SUZUKI, ITSUKO SUZUKI, SUNY-Binghamton, MOTOMIHIRO MATSUIURA, Fukui University of Technology, Japan — Memory interference effects of aging behavior in stage-2 CoCl2 GIC (Tcu = 8.9 K and Tjd = 6.9 K)1,2 have been studied by low frequency (f = 0.1 Hz) AC magnetic susceptibility and genuine thermoremanent magnetization experiments. When the system is aged at multiple stop temperatures (Ts) for wait times (typically tw = 5.0 × 104 s) during a zero-field cooling (ZFC) protocol, the AC magnetic susceptibility exhibits multiple aging holes (dips) at the stop temperatures (Ts ≤ Tcu) on reheating. The depth of the aging hole at Ts = 6.0 K is logarithmically proportional to the wait time. The depth of the aging hole (for the same Tw) exhibits a local maximum at 6.5 K just below Tcu. It drastically decreases with increasing temperature and reduces to zero above Tcu. The genuine thermoremanent magnetization (TRM) measurement also indicates that the memory of the specific spin configurations imprinted at multiple stop temperatures between Tcu and Tjd for a wait time during the field-cooled (FC) protocol can be retrieved on reheating.


4:42PM D41.00012 Experimental Determination of the Heats of Formation for the Ordered Intermetallics in the Fe-Pt System. DAVID BERRY, KATAYUN BARMAK, Carnegie Mellon University, YSELA CHIARI, The Florida State University — Accurate heats of formation are necessary to examine phase stability and to aid in the modeling of phase transitions. However, most reported heats of formation, particularly for intermetallic compounds, are available only as the result of theoretical calculations with little or no experimental verification. For the Fe-Pt system, in which a phase transition from the disordered A1 phase to the ordered L10 phase is of great current interest for application in ultrahigh density magnetic recording media, only a few sets of calculated heats of formation are available, for which there is sizable disagreement. Using non-isothermal differential scanning calorimetry (DSC) of sputter-deposited multilayer thin films, the heats of formation of the ordered intermetallic phases, namely L10 Fe3Pt, and L11 FePt, are measured. These values are then compared with the first principles calculated values available in the literature, where there is good qualitative agreement; however, all of the calculated values have underestimated the total heats of formation.

4:54PM D41.00013 Resistivity, transverse magnetoresistance and Hall effect induced by electron-surface scattering on thin gold films deposited onto preheated mica substrates under high vacuum. RAUL C. MUNOZ, JUAN P. GARCIA, RICARDO HENRIQUEZ, GERMAN KREMER, LUIS MORAGA, Department of Physics, University of Chile — We report measurements of the resistivity ρ, transverse magnetoresistance Δρ/ρ and Hall effect carried out on 4 gold films (thickness of 69, 93, 150 and 185 nm) evaporated onto mica substrates under high vacuum, where the signal is primarily determined by electron-surface scattering. The experiments were performed at low temperatures T (4K ≤ T ≤ 50K) under high magnetic field strengths B (1.5 T ≤ B ≤ 9 T). ρ, Δρ/ρ and the Hall tangent tan(θ) = E_H/E_L (E_H for the transverse Hall field, E_L for the longitudinal field) depend on film thickness. Sondheimer’s theory predicts ρ and tan(θ), but leads to Δρ/ρ one order of magnitude smaller than observed. Calecki’s model predicts ρ and tan(θ), but leads to Δρ/ρ several orders of magnitude smaller than observed. The failure of current theories to predict all 3 transport coefficients is the first compelling evidence pointing to the need of a new, fresh theory to describe size effects arising from electron-surface scattering in metallic films in the presence of a magnetic field. Work funded by FONDECYT 1040723.
tension, and temperature are obtained. Entropy using cluster variation method. Phase diagrams describing the location of ordered and disordered phases as functions of interpore distance, surface ordering. More recently, pore self-ordering has also been observed in other material systems. A general framework to understand the self-ordering is still lacking.

Potential as catalysts or molecular sieves. Optoelectronic applications typically require a perfect spatial pore ordering, while chemical applications demand less.

If both molecules are present on the surface, no intermixing occurs. Instead a separation into two porous networks happens after annealing. M. Stoehr et al., Angew. Chem. similar perylene derivative (TAPP), an open quadratic assembly is found on Cu(111), which is not based on temperature-induced modification. If both molecules generated, since in a thermally induced reaction the end groups of the molecule are modified and it can then act as both a H-bond donor and acceptor. For a

STOEHR, MARKUS WAHL, TOMAS SAMUELY, University of Basel, Switzerland, THOMAS A. JUNG, Paul-Scherrer-Institute, Switzerland, LUTZ H. GADE, University of Heidelberg, Germany — Self-assembly of molecules on surfaces directed by supramolecular interactions has been widely explored. The perylene derivative (DPDI) we analyzed is modified on the surface in order to achieve self-assemblies. This modification is temperature-induced, thus providing an additional feature to the control of self-assemblies in contrast to usual approaches that make use of molecular properties already inherent to the molecules. Thin films of DPDI were prepared on Cu(111) and investigated with STM. Depending on the coverage before annealing, three different H-bond assemblies are generated, since in a thermally induced reaction the end groups of the molecule are modified and it can then act as both a H-bond donor and acceptor. For a similar perylene derivative (TAPP), an open quadradic assembly is found on Cu(111), which is not based on temperature-induced modification. If both molecules are present on the surface, no intermixing occurs. Instead a separation into two porous networks happens after annealing. M. Stoehr et al., Angew. Chem. Int. Ed. 44 (2005) 7394
3:30PM D42.00006 Characterization of molecular linkages of Zeolite microcrystal assembly. HEEJU LEE, Dept. of Physics, Sogang University, Korea, JIN SEON PARK, Dept. of Chemistry, Sogang University, Korea, KYUNG BYUNG YOON, Dept. of Chemistry & Interdisciplinary Program of Integrated Biotechnology, Sogang University, Korea, HYUNJUNG KIM, Dept. of Physics & Interdisciplinary Program of Integrated Biotechnology, Sogang University, Korea — We have measured x-ray reflectivity curves of silicate-1 microcrystal (MC) monolayers on Si wafers using two different types of molecular linkages, namely, through chloropropyl (CP) groups and through CP/polyethylene imine/CP groups. While the scanning electron microscope images of the two MC monolayers are indistinguishable of molecular linkage between the monolayers and the substrate, their reflectivity curves are distinctively different, despite the fact that the thicknesses of the molecular linkage layers (~1-2 nm) are negligibly small compared to the thickness of MC monolayers (~320 nm). We demonstrated that x-ray reflectivity is a very useful tool for the characterization of very thin layers of molecular linkages existing between much thicker MC monolayers and the substrate.

1Supported by Korea Science & Engineering Foundation and Seoul Research & Business Development Program (10816).

3:42PM D42.00007 Determination of the hyperpolarizability components of hemicyanine dyes by measuring the anisotropic fluorescence and second harmonic of the dyes uniformly aligned within zeolite channels. DOSEOK KIM, Department of Physics and Interdisciplinary Program of Integrated Biotechnology, Sogang University, TAEKYU SHIM, Department of Physics, Sogang University, MYOUNGHEE LEE, Department of Chemistry, Sogang University, BUMKU RHEE, HYEONSIK CHEONG, Department of Physics, Sogang University, HYUNSUNG KIM, KYUNGBYUNG YOON, Department of Chemistry, Sogang University — Unidirectional ensemble of hemicyanine molecules was prepared by inserting the molecules into the vertical channels of a uniformly-oriented zeolite (silicate-1) film grown on a glass substrate. Fluorescence from this sample excited with light polarized along the vertical channel was 50 times larger than that excited with light polarized orthogonal to the vertical channel direction. This vertically aligned hemicyanine dyes were used to determine the ratio of the molecular hyperpolarizability components $\beta_{xx}/\beta_{zz}$ of hemicyanine.

3:54PM D42.00008 Orientational Order and Hyperpolarizability of Nonlinear Chromophore Molecules Supported in Amphilicic 4-Helix Bundle Peptides. GRAZIA GONELLA, ANDREY TRONIN, MICHAEL J. THERIEN, HAI-LUNG DAI, J. KENT BLASIE, Department of Chemistry, University of Pennsylvania — The designed nonlinear optical chromophore, (Polypropylyl)Ruthenium-(Porphinato)Zinc(II) (Ru-PZn), incorporated in a monolayer of amphilicic 4-helix bundle peptides which is used to provide control of the chromophore orientational order on a silica substrate, has been examined by optical Second Harmonic Generation (SHG). The single monolayer of the H6H2O AP0 [1] peptide covalently attached to an alkylated silica surface with thiol end groups can be used to host and support Ru-PZn cofactor. It has been found that the cofactor's hyperpolarizability tensor is dominated by its component along the conjugation axis as suggested by Karki et al. for similar systems [2]. The tilt angle of the principal symmetry axis of the chromophore molecule from the surface normal has been determined as well as the absolute magnitude of the molecular nonlinear polarizability through comparison with a quartz crystal.


4:06PM D42.00009 Ab initio simulations of alkyl-terminated Si(001) surfaces. GIANCARLO CICERO, Physics Department, Politecnico di Torino, Torino — Self assembled monolayers (SAMs) are ordered molecular assemblies formed by the adsorption of an active surfactant on a solid surface. The interest in the area of self-assembly, and specifically in SAMs, stems partially from their perceived relevance to science and technology. In contrast to ultrathin films made by, for example, chemical vapour deposition, SAMs are highly ordered and oriented and can incorporate a wide range of groups both in the molecular chain and at the chain termination. Therefore, a variety of surfaces with specific interactions can be produced with fine chemical control. In particular, SAM are used in cantilever based detection, as the first step towards the realization of surfaces with specific sensing properties. Understanding how the surface stress and the mechanical properties of a cantilever change upon functionalization is fundamental to achieve accurate quantitative analysis. Here we present ab initio simulations of SAM formation on Si(001) surface to make contact with some recent experimental results [1], in which well packed and ordered alkyl-terminated silicon surfaces were obtained. We will show how the Si(001) surface stress and its mechanical properties (elastic constants) change when organic molecules are attached to it. In particular we will discuss the effect of increasing the surface coverage and the length of the alkyl chain used for the functionalization process. [1] Cerofolini G. F. Semicond. Sci. Technol. 18, 423-429 (2003).

4:18PM D42.00010 Structure and morphology of (111) textured Au/Co/Au trilayers grown on glass by MBE. DIVINE KUMAH, Applied Physics Department, University of Michigan, J.R. SKUZA, Physics and Astronomy Department, University of Toledo, A. CEBOLLADA, C. CLEVARO, J.M. GARCIA MARTIN, Instituto de Microelectronic de Madrid-IMIM, R.A. LUKASZEW, Physics and Astronomy Department, University of Toledo, ROY CLARKE, Applied Physics Program, University of Michigan — A complete structural and morphological study as a function of Co thickness is presented in a series of Au/Co/Au trilayers grown by MBE on glass substrates. A combined AFM, RHEED, SAXRR and XRD characterization allows determining the optimum deposition conditions that lead to the fabrication of highly textured, flat and continuous layered structures. Development of (111) texture upon annealing the Au layer grown on glass is followed in situ using RHEED. High crystalline quality is confirmed by XRD measurements. A simultaneous in-plane and out-of-plane Co lattice expansion is observed for the thinnest Co layers, converging to bulk values for thickest Co layers. Fluorescence from this sample excited with light polarized along the vertical channel was 50 times larger than that excited with light polarized orthogonal to the vertical channel direction. This vertically aligned hemicyanine dyes were used to determine the ratio of the molecular hyperpolarizability components $\beta_{xx}/\beta_{zz}$ of hemicyanine.

1Supported by Korea Science & Engineering Foundation and Seoul Research & Business Development Program (10816).

4:30PM D42.00011 Silicon-on-insulator for symmetry-converted growth. Y. FUJIKAWA, Y. YAMADA-TAKAMURA, G. YOSHIKAWA, Institute for Materials Research, Tohoku University, T. ONO, M. ESASHI, Faculty of Engineering, Tohoku University, P. ZHANG, M. G. LAGALLY, University of Wisconsin-Madison, T. SAKURAI, Institute for Materials Research, Tohoku University — Because of its well-established processability, good electronic-transport properties, and ability to form a stable insulating oxide, silicon will remain the essential semiconductor for fabrication of electronic devices. Most device fabrication uses Si(001) and hence most of fundamental research, including heteroepitaxy and integration, has focused on Si(001), a square lattice. Materials having 3- or 6-fold symmetries, a major and important class with key properties, have intrinsic difficulty in their growth on Si(001) because the symmetry mismatch induces polycrystallization at the interface and degrades the film quality. We present a general solution for this long-standing problem that allows maintaining the Si(001) bulk material for those aspects of device fabrication that require it while making possible the growth of 3-fold symmetric structures. We utilize silicon-on-insulator (SOI) in which Si(111) is bonded to Si (001). A 14 nm-thick Si(111) template layer is bonded to Si(001) via the buried oxide. Using the surface preparation method recently developed for the Si(001)-SOI surface, this SOI structure provides a uniform Si(111)-7x7 clean surface. Wurtzite GaN is grown directly on this SOI structure, forming of uniform N-polar film.
4:42PM D42.00012 Nanotube Formation from Self-Bending Nanofilms Driven by Atomic-scale Surface Stress Imbalance1, JI ZANG, MINGHUAU HUANG, FENG LIU, Department of Materials Science and Engineering, University of Utah, Salt Lake City, UT 84112 — We present a novel mechanism for fabricating nanotubes by self-bending of nanofilms under intrinsic surface stress imbalance due to surface reconstruction. A freestanding Si nanofilm may spontaneously bend itself into a nanotube without external stress load, and a bilayer SiGe nanofilm may bend into a nanotube with Ge as the inner layer, opposite of the normal bending configuration defined by misfit strain. Such rolled-up nanotubes can accommodate a high level of strain, even beyond the magnitude of lattice mismatch, greatly modifying the tube electronic and optoelectronic properties.

1This work is supported by DOE.

4:54PM D42.00013 Formation of metallic periodic nanostructures by spontaneous oscillation in self-organized electrorcrystallization, MU WANG, RUWEN PENG, GUOBIN MA, XIPING HAO, NAIBEN MING, Dept. Phys., Nanjing University — A unique electrodoposition system is designed to self-organize metallic periodic nanostructures on the surface of solid substrate, which consists of an ultrathin electrolyte layer about 300 nm in thickness. In this system the metal electrodopositions (copper, cobalt, zinc and silver) are formed robustly on the solid substrate (glass, silicon, or glass plates), possess considerably low branching rate, and usually cover with periodic metal/metal oxide nano-nodules. Both potentiostatic and galvanostatic modes can be applied to generate such structures. Following issues are focused in this presentation: (1) The mechanism for the formation of the periodic nanostructures on the films; (2) The experimental conditions to control the periodicity of these periodic spatio-temporal structures; (3) The electric properties of this nano-nodules chains.

References:

Monday, March 5, 2007 2:30PM - 5:30PM —
Session D43 DCMP: Synthesis and Growth of Nanostructured Materials Colorado Convention Center

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2:30PM D43.00001 Detailed Structure Determination of Nanostructures by Low-Energy Electron Diffraction.1, MICHEL VAN HOVE, G.M. GAVAZA, Z.X. YU, City University of Hong Kong, L. TSANG, University of Washington-Seattle, C.H. CHAN, S.Y. TONG, City University of Hong Kong — Detailed structural information of nanostructures (e.g. bond lengths and bond angles) is needed to allow the understanding and prediction of their physical and other properties. To that end we have extended the theoretical capabilities of surface structure determination by Low Energy Electron Diffraction (LEED) to nanostructures. Our new computational method has a compute time that scales as NlogN in terms of the number N of independent atoms, in contrast to N^2 or N^3 typical of conventional LEED calculations of electron multiple scattering. We exhibit the resulting ability to solve detailed nanostructures of different kinds: buckyballs adsorbed on a Cu(111) surface; endohedral and exohedral buckyballs with additional Li or Cu atoms; adsorbed carbon nanotubes; and silicon nanowires. This demonstration of the capability to solve nanostructures should spur the development of experimental methods to measure electron diffraction from nanostructures.

1Funded by RGC grant No. CityU1/02C and DOE.

2:42PM D43.00002 Modeling the Role of Ligands in Controlling the Sizes, Shapes and Supramolecular Ordering of Quantum Dots, MICHAEL TAMBRASCO, SANAT KUMAR, Columbia University, IGAL SZLEIFER, Purdue University — The density of electronic states controls many physical properties of a quantum dot and can be tuned by altering the dot’s size, shape, or composition. In colloidal methods, ligands are used to control quantum dot size, shape, and polydispersity; however, there exists no a-priori means of describing specific conditions that will optimize the synthesis procedure. We apply a mean field theory to study the role of ligands in quantum dot synthesis with particular emphasis on non-spherical shapes. We examine the effects of ligand type and concentration on thermodynamic and structural properties, and compare our results with available data.

2:54PM D43.00003 Migration-influenced island size distribution in interfacial growth, DA-JUN SHU, MU WANG, National Laboratory of Solid State Microstructure and department and Department of Physics, Nanjing University, Nanjing 210093, China — By considering island migration, island interaction and temperature, we demonstrate that distribution of both island size and spatial dispersion on surface can be tuned. It is shown that at lower temperature and stronger inter-island interaction, a narrow size distribution is accompanied by spatial uniformity when island migration is free; yet both size and spatial distribution become random when island migration is forbidden. At higher temperature and weaker inter-island interaction, however, entropy effect dominates, and a narrow size distribution is associated with a fluctuant spatial distribution when island migration is forbidden. These unexpected features are enlightening to fabricate quantum dots where uniformity in both size and spatial distributions are essential.

3:06PM D43.00004 A level-set method for self-organized pattern formation during heteroepitaxial growth, CHRISTIAN RATSCH, UCLA, YOUNG-JU LEE, XIAOBIN NIU, RUSSEL CAFLISCH — We have developed an island dynamics model for heteroepitaxial growth that employs an island dynamics model with the level-set technique in combination with a fully self-consistent elastic model. At every timestep in the simulation, we solve the elastic equations for the entire system. This is possible within our approach because the numerical timestep can be chosen much larger than in an atomistic simulation. At every lattice site strain then changes the local bonding, and thus the potential energy surface for adatoms and the microscopic parameters of the simulation. In particular, strain changes the diffusivity of adatoms and enhances the rate of detachment from island edges. We will show how islands become smaller and more regular upon increasing strain. The reason is that bigger islands are typically more strained than smaller islands, and thus their growth is slowed down. We also present results that show that strain moves the system from layer-by-layer growth to the formation of coherent islands as a mechanism for strain relieve.

3:18PM D43.00005 Phononic Band Gaps in Colloidal Crystals at Hypersonic Frequencies. GEORGE FYTAS, Department of Materials Science and Technology and FORTH, Heraklion, Greece and Max Planck Institute for Polymer Research, Mainz, Germany, WEI CHENG, EUGENIA NUNDE, ULRICH JONAS, Max Planck Institute for Polymer Research, Mainz, Germany, NIKOLAOS STEFANOU, Section of Solid State Physics, University of Athens, Panepistimioupolis, Athens, Greece — The phononic properties of fabricated closed packed fcc colloidal crystals were investigated by high resolution Brillouin light scattering spectroscopy in the GHz frequency range. The dispersion relation has revealed two phononic band gaps: (i) a Bragg—gap occurring at the boundary of the first Brillouin zone and (ii) a hybridization-gap resulting from the interaction of particle eigenmodes with the acoustic mode of the effective medium. Crystallinity is a prerequisite for the appearance only of the Bragg-gap. Depending on the particle size and the speed of sound in the infiltrated fluid, the frequency and the width of the Bragg-gap can be tuned. Since hypersonic crystals can simultaneously exhibit phononic and photonic band gaps in the visible spectral region, the technological applications could range from tunable filters and heat management to acoustic-optical devices.
3:30PM D43.00006 Local crystal structure of iron oxide nanoparticles synthesized from Ferritin, MICHAEL KRISPIN, MARCUS PREISINGER, PETER PFALZER, SIEGFRIED HORN, Institute of Physics, University of Augsburg, 86159 Augsburg, Germany. We have investigated the size dependence of the local crystal structure of nanosized iron oxide by extended x-ray absorption fine structure (EXAFS) at the iron K-edge. Hematite (α-Fe₂O₃) nanoparticles of different diameters were produced by thermal treatment of horse spleen ferritin molecules and rematerialized apo-ferritin molecules, respectively. The structure of these particles was compared to α-Fe₂O₃ and γ-Fe₂O₃ nanoparticles prepared by different routes. EXAFS spectra of the nanoparticles were significantly different from those of iron oxide bulk materials and change systematically as a function of particle diameter, signalling a corresponding evolution of the structure. We show that the Fe–O bond length decreases with decreasing diameter of the particles and with decreasing particle density. This is explained by a core-shell model, in which the fraction of a γ-Fe₂O₃ like particle shell increases while the hematite core decreases with decreasing particle size.

3:42PM D43.00007 Viscoplasticity and granularity in films of colloidal nanocrystals, DONGYUN LEE, SHENGGUO JIA, SARBAJIT BANERJEE, JOZE BEVK, IRVING HERMAN, JEFFREY KYSAR, Materials Research Science and Engineering Center, Columbia University. Thin films composed of colloidal CdSe nanocrystals have been electrophoretically deposited onto Au/Si substrates with thicknesses ranging from 300 to 3200 nm. The mechanical properties of these films have been measured by nanoindentation. Indentation is carried out to 25% of total thickness (less if greater than 300 nm). The total displacement at the end of each test is less than the penetration depth. For the CdSe films, the elastic modulus and hardness are found to be independent of thickness. In addition, the force is held at peak load for up to 20 s to observe the creep behavior of the films. The elastic modulus and hardness of 3.2 nm nanocrystal films are ~10 GPa and ~450 MPa, respectively. Furthermore, after particle cross-linking and partial ligand removal, the films exhibit compaction of the cores. This mechanical response suggests these nanocrystal films have polymeric features that can be attributed to the organic ligands and granular characteristics due to the inorganic cores. Both characteristics have also been confirmed by investigating larger nanocrystal films by removing the capping ligands. This work was supported primarily by the MRSEC Program of the NSF under Award No. DMR-0213574 and by NYSTAR. Nanoindentation studies at the Oak Ridge National Laboratory ShARE User Center were sponsored under DE-AC05-00OR22725.

3:54PM D43.00008 Doping colloidal nanocrystals: the role of surfactants, MAO-HUA DU, STEVEN ERWIN, ALEXANDER EFROS, Naval Research Laboratory. The intentional doping of nanocrystals (NCs) with impurity atoms will be critical to their functioning in a variety of technologies. For NCs grown by colloidal synthesis, doping efforts have been far less successful than for their bulk counterparts. We recently proposed a theoretical model that explains this difference [1]. The central idea is that because the temperatures used in colloidal growth are low (250-300 °C), thermal equilibrium between the NCs and the ligands is not achieved. Instead, the surface of the NCs is modified by chemical equilibrium between the NC surface–ligand and the NC surface–impurity. The binding strength between the surfactant and dopants in solution strongly affects the dopant sticking coefficient on the NC surfaces, and the dopant solubility in solution. We focus on Mn doping of CdSe NCs, and use first-principles calculations to shed light on the competition between dopant–surface, surfactant–surface, and dopant–surfactant interactions. Our findings are consistent with experimental results for Mn incorporation in CdSe NCs. [1] S.C. Erwin, L. Zu, M.I. Hartel, A.L. Efros, T.A. Kennedy, and D.J. Norris. Doping semiconductor nanocrystals. Nature 436, 91 (2005).

4:06PM D43.00009 Accurate structure and size determination of CdSe nanoparticles using PDF analysis, A.S. MASADEH, E.S. BOZIN, P. JUHAS, G. PAGLIA, Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824-1116, A. KARKAMKAR, M.G. KANATZIDIS, Department of Chemistry, Michigan State University, East Lansing, Michigan 48824-1116, S.J.L. BILLINGE, Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824-1116. The atomic pair distribution function (PDF) is total scattering based technique, which includes both Bragg and diffuse scattering, can provide quantitative information about the local structure of the materials at different length scales. The PDF method is used to quantify intermediate-range order and address the size and structure in series of CdSe nanoparticles (NPs), with diameter sizes ranging from 2 to 4 nm, prepared by the methods of Peng et al.¹. The PDF data were collected at the APS, using high energy x-rays. I will discuss how the PDF yields precise structural information about the NPs such as local bonding, atomic structure size of the core, and so on, as a function of NP diameter. For example, the core structure of the measured CdSe NPs was found to possess a well-defined wurtzite structure. The diameter of CdSe NPs extracted from the PDF data is in good agreement with the one obtained from standard methods. (1) Peng et al. J. Am. Chem. Soc. 1998, 120, 5343-5344.

4:18PM D43.00010 Sub-100 nm interferometric lithography realized with table top extreme ultraviolet lasers, MARIO MARCONI, PRZEMYSLAW WACHULAK, DINESHCHANDRA PATEL, Department of Electrical and Computer Engineering, Colorado State University, Fort Collins, CO 80523, USA, MARIA GABRIELA CAPELUTO, Department of Electrical and Computer Engineering, Colorado State University, Fort Collins, CO 80523, USA, NSF ENGINEERING RESEARCH CENTER FOR EXTREME ULTRAVIOLET SCIENCE & TECHNOLOGY TEAM — We demonstrated patternning of arrays of nano-dots over areas of 500 x 500 µm² at the micrometre scale, using high energy x-rays. I will discuss how the PDF yields precise structural information about the NPs such as local bonding, atomic structure size of the core, and so on, as a function of NP diameter. For example, the core structure of the measured CdSe NPs was found to possess a well-defined wurtzite structure. The diameter of CdSe NPs extracted from the PDF data is in good agreement with the one obtained form standard methods. (1) Peng et al. J. Am. Chem. Soc. 1998, 120, 5343-5344.

4:30PM D43.00011 Chemical Nanomachining of Si, JEREMY ROBINSON, University of California-Berkeley, Berkeley, CA 94720, PAUL EVANS, University of Wisconsin-Madison, Madison, WI 53706, J. ALEX LIDDLE, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, OSCAN DUBON, University of California-Berkeley, Berkeley, CA 94720. We demonstrate a simple process for chemical nanomachining of reproducible Si nanostuctures. Using a stencil mask containing windows of various geometries, we evaporate Au onto a Si surface rinsed in HF. The pattern formed by the spontaneous oxidation of Si at and around each patterned Au feature serves as a mask for the underlying Si and permits the use of simple wet chemistry to produce highly ordered nanostuctures of diverse shapes including rings, pillars, wires, and nanoropes. Pillars are formed by etching a Si sample patterned with an array of nominally 1 nm-thick Au squares having a side discussion of 200 nm. Remarkably, the Au capped core of these pillars can be removed by briefly rinsing the Au-patterned sample with HF prior to etching with KOH. When the Au-squares are sufficiently close together, the anodic oxide patterns surrounding the Au squares overlap to form a continuous surface oxide. Etching in this case with HF followed by KOH produces a continuous Si film with holes. Thus, this unique catalyzed patterning process opens the door for the rapid, parallel fabrication of a variety of nanostructures that are unfeasible or impractical to fabricate with traditional processing routes.

4:42PM D43.00012 Sculpting of Nanopores in Silicon-Nitride Membranes, KRISTIN LUCAS, JEFFREY L. WASSERMAN, SOO HYUNG LEE, NINA MARKOVIC, Johns Hopkins University. Fabrication of controllable-diameter nanopores in a suspended membrane is of great interest for dynamic stencil deposition techniques, as well as DNA sequencing and other applications. We have developed a method for the production of nanopores in silicon nitride membranes. The nanometer-sized hole is produced by focused ion beam or lithographic techniques. By exposing the holes to an electron beam we can shrink the pore diameter down to a few nanometers. We can also produce complex pore shapes through selective sculpting of the pore. We will discuss the details of the process and its applications.
This work reflects a collaboration with M.P. Lilly, K.B. Cooper, I.B. Spielman, M. Kellogg, L.A. Tracy, L.N. Pfeiffer, and K.W. West.

which the broken symmetry phase can equivalently be described as a pseudospin ferromagnet or an (imperfect) excitonic superfluid.

low temperatures when currents are driven in opposite directions through the two layers. These, and other observations are broadly consistent with theories in

the bilayer equals the degeneracy of a single Landau level, an unusual phase appears at small layer separation. This phase possesses a novel broken symmetry,

charge density modulation. Orientational ordering of small striped domains at low temperatures accounts for the resistive anisotropy and is reminiscent of the

systems near half-filling of highly excited Landau levels new states characterized by a massive anisotropy in the electrical resistivity of the sample are observed

from flat plane, porous structure, and pebble structure to island structure as the annealing temperature increases.

This work was supported by AFOSR MURI # F49620-02-1-0288.

Monday, March 5, 2007 8:00PM - 9:48PM – Session G1 DCMP: 50 Years of BCS Theory , Adam039;s Mark Plaza Ballrooms A-B

8:00PM G1.00001 The Impact of the BCS Theory on Condensed Matter Physics , DOUGLAS J. SCALAPINO, University of California, Santa Barbara — Fifty years after the BCS theory revolutionized our understanding of superconductivity it is interesting to look at the broad impact it has had and continues to have on physics. Here, I have been asked to focus on the importance of this seminal work for the field of condensed matter physics.

8:36PM G1.00002 The Impact of the BCS Theory on 50 years of Superconductivity and Condensed Matter Physics , JOHN M. ROWELL, School of Materials, Arizona State University, Tempe AZ — The existence of supercurrents and of an energy gap in superconductors, known before 1957, was explained by Bardeen, Cooper and Schrieffer by proposing that electrons were paired through an interaction with phonons of the lattice of the material. These central ideas, a supercurrent of pairs, and a pairing interaction creating an energy gap, quickly became pervasive in experimental research in superconductivity, and over time had impact much more broadly in condensed-matter physics and beyond. In this talk, I will attempt to illustrate the influence of these ideas, by choosing experiments that I was either involved in exploring, or that appeal to me because of their novelty.

9:12PM G1.00003 BCS – from Atoms and Nuclei to the Cosmos , GORDON BAYM, University of Illinois at Urbana-Champaign — BCS theory has had a profound impact on physics well beyond laboratory superconductors and superfluids. This talk will describe the influence of the theory — spanning more than 20 decades of energy scales — from nuclear physics, neutron stars, and quark matter, to ultracold trapped atoms.

Tuesday, March 6, 2007 8:00AM - 10:24AM – Session H1 DCMP: DCMP Prize Session , Colorado Convention Center Four Seasons 2-3

8:00AM H1.00001 Beyond the Quantum Hall Effect: New Phases of 2D Electrons at High Magnetic Field , JAMES EISENSTEIN, Caltech — In this talk I will discuss recent experiments on high mobility single and double layer 2D electron systems in which collective phases lying outside the usual quantum Hall effect paradigm have been detected and studied. For example, in single layer 2D systems near half-filling of highly excited Landau levels new states characterized by a massive anisotropy in the electrical resistivity of the sample are observed at very low temperature. The anisotropy has been widely interpreted as the signature of a new class of correlated electron phases which incorporate a stripe-like charge density modulation. Orientational ordering of small striped domains at low temperatures accounts for the resistive anisotropy and is reminiscent of the isotropic-nematic phase transition in classical liquid crystals. Double layer 2D electron systems possess collective phases not present in single layer systems. In particular, when the total number of electrons in the bilayer equals the degeneracy of a single Landau level, an unusual phase appears at small layer separation. This phase possesses a novel broken symmetry, spontaneous interlayer phase coherence, which has a number of dramatic experimental signatures. The interlayer tunneling conductance develops a strong and very sharp resonance around zero bias resembling the dc Josephson effect. At the same time, both the longitudinal and Hall resistances of the sample vanish at low temperatures when currents are driven in opposite directions through the two layers. These, and other observations are broadly consistent with theories in which the broken symmetry phase can equivalently be described as a pseudospin ferromagnet or an (imperfect) excitonic superfluid.

This work reflects a collaboration with M.P. Lilly, K.B. Cooper, I.B. Spielman, M. Kellogg, L.A. Tracy, L.N. Pfeiffer, and K.W. West.
8:36AM H1.00002 Off-Diagonal Long-Range Order and Collective Excitations in the Fractional Quantum Hall Effect. STEVEN GIRVIN, Yale University — The experimental discovery of the fractional quantum Hall effect was a stunning surprise which came to be understood in terms of a novel state of matter in which strongly correlated electrons acquire a new and unprecedented type of collective quantum order. The mystery of superconductivity was first understood macroscopically in terms of Ginsburg-Landau effective theory before the microscopic BCS theory was developed. Here the historical order was reversed. Laughlin discovered his essentially exact microscopic wave function and only subsequently did we begin to understand its implications in terms of a new type of off-diagonal long-range order and an effective Chern-Simons field theory for composite particles carrying magnetic flux. In this gauge theory, the fact that Laughlin’s quasi-particle excitations carry sharply quantized fractional charge could be understood as analogous to sharp flux quantization in a superconductor. The fact these vortex excitations have finite energy could be understood as the result of magnetic screening by the gauge field. In addition to discussing this macroscopic picture of the FQHE, I will also discuss the microscopic wave function that Allan MacDonald and I developed in collaboration with Phil Platzman which accurately describes the gapped magneto-phonon and magneto-roton collective excitations of the system.

9:12AM H1.00003 Oliver E. Buckley Prize Talk. ALLAN MACDONALD, Univ of Texas — No abstract available.

9:48AM H1.00004 Atom Chains at Surfaces: A Playground for Low-Dimensional Physics. FRANZ HIMPSEL, University of Wisconsin Madison — One-dimensional physics is particularly elegant because of its mathematical transparency. However, it is not easy to realize a one-dimensional system experimentally. Using self-assembly techniques, it has become possible to produce atomic chain structures at silicon surfaces and to control their dimensionality, their band filling, and their magnetic moment [1]. The atoms are locked to the surface, but metallic electrons are decoupled from the substrate due to the band gap of silicon. In a sense, these are the ultimate nanowires, each consisting of a single chain of orbitals. Angle-resolved photoemission reveals surprising features, such as a fractional band filling [2], a spin-splitting at a non-magnetic surface [3], and the one-dimensional analog of stripes (alternating metallic and semiconducting sections).


Tuesday, March 6, 2007 8:00AM - 11:00AM – Session H3 DCMP: Anomalous Hall Effect: Theory and Experiments

8:00AM H3.00001 Intrinsic vs. extrinsic mechanisms of anomalous Hall effect. SHIGEKI ONODA, CREST, Department of Applied Physics, University of Tokyo — Anomalous Hall effect (AHE) in ferromagnets has been a fundamental and intriguing issue in condensed-matter physics. Various mechanisms have been proposed, including the Karpplus-Luttinger’s band intrinsic mechanism, and extrinsic skew-scattering and side-jump mechanisms. However, the controversy on the mechanism has not been resolved yet. In this talk, a unified theory of the anomalous Hall effect (AHE) is presented for multi-band ferromagnetic metallic systems with dilute impurities [1], using the gauge-covariant formalism for the Keldysh Green’s function that Allan MacDonald and I developed in collaboration with Phil Platzman which accurately describes the gapped magneto-phonon and magneto-roton collective excitations of the system.


8:36AM H3.00002 The Anomalous Hall effect in MnSi and Fe$_x$TaS$_2$. MINHYEA LEE, Princeton University — In a high-purity ferromagnet with long carrier lifetime $\tau$, e.g. MnSi, the ordinary Hall conductivity $\sigma_{xy}^H$ can dominate the intrinsic Anomalous Hall effect (AHE) conductivity $\sigma_{xy}^A$. We show that the large magnetoresistance provides a way to separate accurately the two Hall currents. Below $T_C$, we find that the AHE conductivity is strictly proportional to the magnetization $M$, viz. $\sigma_{xy}^A = S_H M$ with a parameter $S_H$ that is independent of both temperature $T$ and field $H$. This implies that $\sigma_{xy}^A$ is strictly independent of $\tau$. In the layered, hard ferromagnet Fe$_x$TaS$_2$, the large coercivity leads to abrupt reversals of $M$ when it switches. We show that this provides an accurate way to separate $\sigma_{xy}^A$ from $\sigma_{xy}^H$. Again, $\sigma_{xy}^A$ is independent of $T$ from 5 to 50 K. We compare the observed constancy at low $T$ with theories for the AHE. We also describe a Hall anomaly recently observed in MnSi under pressure. This anomaly appears to arise from strong sensitivity of the Hall current to the spin texture, possibly reflecting its finite chirality. The dependence of the anomaly to $T$ and $H$ will be reported.

**This work is done in collaboration with Y. Onose, J. G. Checkelsky, E. Morosan, R. J. Cava, Y. Tokura and N. P. Ong.

1 This work was carried out at NIST, Indiana University and Yale University and was supported by the NSF.
we have operated largely in an automated mode, inputting the DFT or Hartree-Fock solutions as trial wave functions. The AF QMC results showed consistently
including Si solid, first- and second-row molecular systems, molecules of heavier post-d elements, transition-metal systems, and ultra-cold atomic gases. In these
from standard electronic structure methods into a many-body QMC framework. We have demonstrated this method with calculations in close to 100 systems,
random walk paths to control the sign/phase problem, which has shown to be very accurate even with simple mean-field solutions as the constraining trial
"Entanglement" of the different field configurations leads to random walks in Slater determinant space. We formulate an approximate constraint on the
expression is carried out for the material CuCr$_2$Se$_4$, obtaining quantitative agreement with a recent experiment. This work is done in collaboration with
the anomalous Hall effect that suggest that even for stoichiometric ferromagnetic crystals, such as those studied in this work, the intrinsic Hall conductivity is
anomalous Hall conductivity depends linearly on the magnetization, and linear (in field) magnetoresistance. Based on a general, finite-temperature, formula for orbital magnetization, we
important role in the dynamics of Bloch electrons. For instance, the electron will acquire an anomalous velocity term transverse to the applied electric field,
are able to develop a satisfactory theory for anomalous transport in ferromagnets driven by statistical forces (the gradient of temperature or chemical potential).
Based on a general, finite-temperature, formula for orbital magnetization, we
giving rise to an intrinsic contribution to the anomalous Hall effect. We have recently discovered that the Berry phase also modifies the phase-space density
from the Berry curvature of the Bloch states using first-principles methods. The intrinsic anomalous Hall conductivity is mainly caused by the mixing of the AHE with the magneto-resistance and
differential susceptibility. This work was done in collaboration with Y. Yao, Di Xiao, Q. Niu, and H.H. Weiting.

9:12AM H3.00003 Investigation of the Anomalous Hall Effect in Three Unusual Ferromagnets
BRIAN SALES, Oak Ridge National Laboratory — The Hall resistivity ($\rho_{xy}$), resistivity ($\rho_{xx}$), and magnetization of three ferromagnetic materials are investigated as a function of magnetic field and temperature [1]. The three ferromagnets, EuFe$_x$Sb$_{12}$ ($T_c=84$ K), Yb$_{14}$Mn$_{30}$Sb$_{11}$ ($T_c\approx 53$ K), and Eu$_8$Ga$_{16}$Ge$_{30}$ ($T_c\approx 36$ K) are Zintl compounds with carrier concentrations between $1 \times 10^{22}$ cm$^{-3}$ and $3.5 \times 10^{21}$ cm$^{-3}$. The relative decrease in $\rho_{xx}$ below $T_c$ ($\rho_{xx}(T_c)/\rho_{xx}(2 K)$) is 28, 6.5, and 1.3 for EuFe$_x$Sb$_{12}$, Yb$_{14}$Mn$_{30}$Sb$_{11}$, and Eu$_8$Ga$_{16}$Ge$_{30}$ respectively. The low carrier concentrations coupled with low magnetic anisotropies allow a relatively clean zero-field separation between the anomalous ($\rho_{xy}$), and normal contributions to the measured Hall resistivity. For each compound the anomalous contribution in the zero field limit is fit to $\rho_{xy}=\sigma_{xy}/\rho_{xx}$ for temperatures $T<T_c$. The anomalous Hall conductivity, $\sigma_{xy}$, is $-220 \pm 5$ ($\Omega^{-1}$ cm$^{-1}$), $147 \pm 1$ ($\Omega^{-1}$ cm$^{-1}$), and $28 \pm 3$ ($\Omega^{-1}$ cm$^{-1}$) for EuFe$_x$Sb$_{12}$, Yb$_{14}$Mn$_{30}$Sb$_{11}$, and Eu$_8$Ga$_{16}$Ge$_{30}$ respectively and is independent of temperature for $T<T_c$, if the change in spontaneous magnetization (order parameter) with temperature is taken into account. These data appear to be consistent with recent theories of the anomalous Hall effect that suggest that even for stoichiometric ferromagnetic crystals, such as those studied in this work, the intrinsic Hall conductivity is finite at $T=0$ that can be calculated from the electronic structure. New measurements on single crystals of the tetragonal compound Yb$_{14}$Mn$_{30}$Sb$_{11}$, however, indicate that the intrinsic Hall conductivity can change sign, depending on the direction of the current and magnetic field with respect to the crystallographic axes. These new results will also be discussed within the context of recent theories. Research was done in collaboration with Rongying Jin, David Mandrus and Peter Khalifah.

9:48AM H3.00004 Ordinary and anomalous Hall effects of ferromagnetic Mn$_5$Ge$_3$ CHANGGAN ZENG, Department of Physics and Astronomy, University of Tennessee — It is well known that in ferromagnetic materials, the Hall effect includes two
contributions: the ordinary Hall effect (OHE), which is proportional to the applied magnetic field, and the anomalous Hall effect (AHE), which originates from the
magnetization of the material. Although both phenomena have been thoroughly studied, there are still questions about the origins of both OHE and AHE in ferromagnetic materials with complicated band structures. Using ferromagnetic Mn$_5$Ge$_3$ thin films as an example, we investigate the Hall effect experimentally and theoretically. We have separated the intrinsic and extrinsic contributions to the experimental AHE and calculated the intrinsic anomalous Hall conductivity from the Berry curvature of the Bloch states using first-principles methods. The intrinsic anomalous Hall conductivity depends linearly on the magnetization, which can be understood from the long-wavelength fluctuations of the spin orientation at finite temperatures. The quantitative agreement between theory and experiment is remarkably good, not only near 0 K but also at finite temperatures, up to about 240 K ($0.8 T_c$) [1]. The measured ordinary Hall coefficient is found to change its sign as a function of temperature. From a detailed analysis, which includes magneto-resistance measurements, magnetic characterization, and first-principles calculations, we establish that the sign change of the OHE is mainly caused by the mixing of the AHE with the magneto-resistance and
differential susceptibility. This work was done in collaboration with Y. Yao, Di Xiao, Q. Niu, and H.H. Weiting.

10:24AM H3.00005 Berry phase, Orbital Magnetization, and Anomalous Hall/Nernst Effect . DI XIAO, Department of Physics, The University of Texas at Austin — It is now well recognized that the Berry phase of the electronic wave function plays an important role in the dynamics of Bloch electrons. For instance, the electron will acquire an anomalous velocity term transverse to the applied electric field, giving rise to an anomalous contribution to the Hall effect. We have recently discovered that the Berry phase also modifies the phase-space density of states in the presence of a magnetic field. This surprising result has a number of implications, such as a field-dependent Fermi sea volume, Berry phase correction to the orbital magnetization, and linear (in field) magnetoresistance. Based on a general, finite-temperature, formula for orbital magnetization, we are able to develop a satisfactory theory for anomalous transport in ferromagnets driven by statistical forces (the gradient of temperature or chemical potential). Here a charge Hall current arises from the Berry-phase correction to the orbital magnetization rather than from the anomalous velocity, which does not exist in the absence of a mechanical force. We provide an explicit expression for the off-diagonal thermoelectric conductivity, establish the Mott relation between the anomalous Nernst and Hall effects, and reaffirm the Onsager relation between reciprocal thermoelectric conductivities. A first-principles evaluation of our expression is carried out for the material CuCr$_2$Se$_4$-Br$_x$, obtaining quantitative agreement with a recent experiment. This work is done in collaboration with Q. Niu, J.-R. Shi, Y.-G Yao, Z. Fang.
3. Y. Yao, et. al., cond-mat/0609714.

Tuesday, March 6, 2007 8:00AM - 11:00AM –
Session H4 DCOMP DCMP DMP: Recent Advances in quantum Monte Carlo Simulations Colorado Convention Center Korbel 2B-3B

8:00AM H4.00001 Recent advances in auxiliary-field methods — simulations in lattice models and real materials1. SHIWEI ZHANG, College of William and Mary — We have developed an auxiliary-field (AF) quantum Monte Carlo (QMC) method for many-body simulations. The method takes the form of a linear superposition of independent-particle calculations in fluctuating external fields. "Entanglement" of the different field configurations leads to random walks in Slater determinant space. We formulate an approximate constraint on the random walk paths to control the sign-phase problem, which has shown to be very accurate even with simple mean-field solutions as the constraining trial wave function. The same method can be applied to both simplified lattice models and real materials. For realistic electronic Hamiltonians, each random walk stream resembles a density-functional theory (DFT) calculation in random local fields. Thus, the AF QMC method can directly import existing technology from standard electronic structure methods into a many-body QMC framework. We have demonstrated this method with calculations in close to 100 systems, including Si solid, first- and second-row molecular systems, molecules of heavier post-d elements, transition-metal systems, and ultra-cold atomic gases. In these we have operated largely in an automated mode, inputting the DFT or Hartree-Fock solutions as trial wave functions. The AF QMC results showed consistently good agreement with near-exact quantum chemistry results and/or experiment. I will also discuss additional algorithmic advances which can further improve the method in strongly correlated systems. Supported by ARO, NSF, ONR, and DOE-cmsn.
1In collaboration with W. A. Al-Saud, Henry Krakauer, and Wirawan Purwanto
variational parameters are consistently optimized during the ionic dynamics. \[ \approx \] forces, namely determined by QMC with very short runs. This allows us to simulate finite temperature systems (function introduced by P.W. Anderson in the context of High-Tc superconductivity[2]). For instance, by means of this paradigm, it has been possible to perform a stochastic approach such as QMC. In this way it is possible to describe very accurately the electronic correlation by a first principle many-body wave function, optimization of strongly correlated variational wave functions, it is now possible to optimize several variational parameters with remarkable efficiency even within the limit, and allows one to take into account efficiently the different length scales in the system. Another advantage of this framework is the possibility to include non-local potentials in a consistent variational scheme, substantially improving both the accuracy and the computational stability upon previous non-variational diffusion Monte Carlo approaches. However, we have recently shown[3] that also the standard diffusion Monte Carlo algorithm can be made stable and variational even in the presence of non-local pseudopotentials, by including a non-local discrete process in the diffusion operator. This work can open the route for even more reliable and accurate electronic ground state calculations using diffusion Monte Carlo methods.

1 This work was partially supported by the NSF grant DMR-0404853

9:12AM H4.00003 Pfaffian wave functions and topology of fermion nodes, LUBOS MITAS, North Carolina State University — Pfaffian is defined as a signed sum of all pair partitions of even number of elements and it can be viewed as a nontrivial generalization of determinant. Pfaffian enables to define the simplest possible antisymmetric wave function based on pair spinorital(s) and therefore represents a pairing generalization of the Slater determinant of one-particle orbitals. Pfaffians actually accomodate several types of pairing wave functions, for example, one special case is the Bardeen-Cooper- Schrieffer wave function. Using this platform we propose pfaffian wave functions with simultaneous pairings both in singlet and triplet channels and we benchmark their performance in fixed-node quantum Monte Carlo. We implement Gaussian elimination-like algorithm which enables to calculate pfaffians with efficiency similar to calculation of determinants. For a testing set of first row atoms and molecules we show that single pfaffians provide correlation energies systematically at the level of about 95%. Linear combinations of small number of pfaffians recover another fraction of the missing correlation energy comparable to significantly larger determinantal expansions. In addition, we show that pfaffians possess an important property of fermionic wave functions, namely, the minimal number of two nodal domains defined by fermion nodes. This is related to the proof that under rather general conditions closed-shell ground states are Pfaffian wave functions of fermionic systems in d>1 have two nodal domains for arbitrary system size. The explicit proofs cover a number of paradigmatic models such as fermions on a sphere surface, in a periodic box, atomic states, etc, and we discuss the implications of this on efficient construction of wave functions and on several types of many-body effects. Supported by NSF and done in collaboration with M. Bajdich, L.K. Wagner, G. Drobny, and K.E Schmidt. Refs: L. Mitas, PRL 96, 240402 (2006); L. Mitas, cond-mat/0605550; M. Bajdich et al, PRL 96, 130201 (2006); cond-mat/0610850.

9:48AM H4.00004 QMC simulations using backflow correlated wave functions, RICHARD NEEDS, University of Cambridge — An inhomogeneous backflow transformation for many-particle wave functions is presented and applied to electrons in atoms, molecules, and solids. Backflow transformations are compact parametrizations, by which we mean that the number of parameters required to retrieve a given fraction of the correlation energy increases only slowly with system size. We report variational and diffusion quantum Monte Carlo (VMC and DMC) energies for a number of systems and study the computational cost of using backflow wave functions. Backflow transformations alter the nodal surface of the wave function and can therefore be used to reduce the fixed-node error in DMC calculations. Applications to the homogeneous electron gas, the all-electron lithium atom and dimer, and carbon atom and dimer, and pseudopotential calculations for the carbon atom and dimer and carbon diamond are presented. When the initial nodal surface is reasonably accurate, backflow appears to do an excellent job in improving the VMC energy and correcting the remaining errors in the nodal surface. When the initial nodal surface is poor, however, backflow is apparently incapable of making the gross changes to the nodal surface required to correct the flaws, although it still normally lowers both the VMC and DMC energies significantly. Overall, we find that inhomogeneous backflow transformations can provide a substantial increase in the amount of correlation energy retrieved within VMC and DMC calculations. This approach is of considerable generality as it is successful in metals and in insulators, and in large and small systems. Backflow transformations can readily be used with pairing wave functions, and this approach could yield significant improvements when a wave function consisting of a single determinant of one-particle orbitals is a poor starting point.

10:24AM H4.00005 Resonating Valence Bond wavefunctions for electronic simulations, SANDRO SORELLA, Democritos National Simulation Centre and SISSA — We discuss several progress for the simulation of strongly correlated electrons, based on an efficient implementation of the Resonating Valence Bond (RVB) theory with Quantum Monte Carlo (QMC). Due to very important advances[1] in the energy optimization of strongly correlated variational wave functions, it is now possible to optimize several variational parameters with remarkable efficiency even within a stochastic approach such as QMC. In this way it is possible to describe very accurately the electronic correlation by a first principle many-body wave function, that can be extended to fairly large electronic systems. Indeed a remarkable improvement of the Hartree-Fock theory is provided by the so called RVB wave function introduced by P.W. Anderson in the context of High-Tc superconductivity[2]. For instance, by means of this paradigm, it has been possible to perform a realistic and accurate simulation of the benzene dimer, where we have found that the RVB correlation of the benzene ring plays a crucial role in the dimer bonding[3,4]. Finally we consider the still controversial low-temperature and high-pressure phase diagram of Hydrogen by using the same RVB wavefunction. We use a novel second order Langevin dynamics by introducing a consistent friction tensor, allowing to remain in thermal equilibrium even with very noisy forces, namely determined by QMC with very short runs. This allows us to simulate finite temperature systems (\( \approx 100 \) H) with very high efficiency, while the variational parameters are consistently optimized during the ionic dynamics.


5 supported by COFIN 2005 and CNR
8:00AM H23.00001 The growth of Manganese wires on Si(100): observation of the sub-monolayer coverage regime with STM, HUI LIU, PETRA REINKE, University of Virginia — The study of thin film magnetic materials and the doping of semiconductors with magnetically active dopant atoms has received increased attention due to their potential applications in magnetic memory devices and spintronics. We observe the deposition of Mn on the Si(100) 2x1 reconstructed surface in the sub-monolayer regime with STM. Short Mn wires with a length of 5 to about 20 atoms are formed an oriented perpendicular to the Si-dimer rows. At higher coverage some Mn wires are anchored with one end of the wire at the edge and extend onto the lower lying surface. The region in between the wires is particularly interesting: if the Mn wire distance is reduced the dimers change their orientation and are tilted, or begin to form zig-zag lines. The wire length and dimer deformation is likely governed by local strain. We will discuss the wire statistics (length, orientation, and position), control of their growth and present first data on the electronic structure of the wires. The growth of Si and Ge overlayers and incorporation of Mn wires in Ge-quantum dots is currently explored.

8:12AM H23.00002 Growth and Characterization of a Combinatorial Array of Magnesium-Aluminum Alloys, DAAD HADDAD, School of Materials Engineering, Purdue University, West Lafayette, IN 47907, CHARLES OLK, Materials and Processes Laboratory, General Motors Research and Development Center, Warren, MI 48091. We have used combinatorial gradient deposition to produce thin films with a wide range of compositions within the Mg-Al alloy system. We have successfully isolated the (Mg$_6$Al$_2$) phase. The importance of understanding the physical properties of the β phase becomes apparent when one realizes the contrary effects associated with its presence in these alloys. The presence of the β phase is desirable for increasing corrosion resistance while undesirable as it generally produces reduced mechanical strength of the alloy. We present details of the growth procedure, as well as structural and compositional characterization.

8:24AM H23.00003 Atomic structures of 13-atom clusters by density functional theory, HSIN-YI CHEN, CHING-MING WEI, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan — The 13-atom cluster structures of the alkaline metals, alkaline earth metals, boron group, 3d, 4d, and 5d transition metals in the periodic table, and Pb are investigated by density functional theory with three kinds of exchange correlation approximation: i) LDA (Local Density Approximation), ii) GGA (Generalized Gradient Approximation) [1], and iii) PBE (Perdew-Burke-Ernzerhof) [2]. The results mainly focus on five 3-D structures: icosahedral, cuboctahedral, hexagonal-closed packed, body-center cubic, decahedral, and the other two layer structures: buckled bilinear (bbp) and garrison-cap bilinear (gpb) structures. Limited by accuracy of exchange correlation approximation, two interesting results are found. The ground states of Cs$_{13}$, Sr$_{13}$, Ba$_{13}$, Sc$_{13}$, Y$_{13}$, La$_{13}$, Ti$_{13}$, Zr$_{13}$, and Hf$_{13}$ are icosahedral structures. The clusters of Ir$_{13}$, Pd$_{13}$, Cu$_{13}$, Ag$_{13}$, and Au$_{13}$ are more favorable for layer structures (i.e. bpb and gpb) than the other five 3-D structures.

9:30AM H23.00004 Length characterization of DNA-wrapped carbon nanotubes using Raman Spectroscopy, SHIN G. CHOU, Pfizer Global Research and Development, HYUNGBIN SON, AUREA ZARE, Massachusetts Institute of Technology, ADO JORIO, Universidade Federal de Minas Gerais, RICHIRO SAITO, Tohoku University, MILDRED DRESSELHAUS, GENE DRESSELHAUS, Massachusetts Institute of Technology — The systematic resonance Raman study has been carried out on DNA-wrapped SWNTs of different lengths using several different values of laser excitation energy. The correlation observed between the intensity ratio of the D-band and G-band features ($I_D/I_G$) and the average nanotube length energies indicates that nanotube length can be used as the dominant structural parameter in Raman characterization, and that the $I_D/I_G$ ratio can be used as a qualitative gauge for estimating the average nanotube length. By systematically varying the laser excitation energy, we have also found that the $I_D/I_G$ ratio strongly depends on whether the tubes are metallic or semiconducting, as well as on the laser excitation energy. Further directions for this research will be presented. The authors gratefully acknowledge support for this research from the National Science Foundation grant DMR-04-05538.

1The authors gratefully acknowledge support for this research from the National Science Foundation grant DMR-04-05538.

8:48AM H23.00005 ABSTRACT WITHDRAWN —

9:00AM H23.00006 Gold Cluster Formation on C$_{60}$ Surfaces: Au-Cluster Beads and Self-Organized Structures, PETRA REINKE, HUI LIU, University of Virginia — Petra Reinke, Hui Liu, Department of Materials Science and Engineering, University of Virginia The investigation of C$_{60}$-Au interaction is central to the advancement of solar cell and nanotechnology applications of C$_{60}$. C$_{60}$ grows in a quasi-layer-by-layer mode on a pristine graphite surface and forms a special surface structure (coexistence of round and fractal islands). The deposition of Au leads to the formation of a complex array of different surface structures, while the basic island structure of the C$_{60}$ is preserved. The Au-clusters nucleate preferentially at the graphite-first fullerene layer islands edge forming beadlike structures. A roughness analysis of the fullerene surface indicates the presence of Au atoms embedded in the fullerene layer, situated in the troughs in between the large molecules. The analysis of the spatial and size distributions of Au clusters provides the basis for the development of a qualitative model which describes the relevant surface processes in the Au-fullerene system. The simultaneous deposition of Au and C$_{60}$ leads to the formation of organized structures, in which Au clusters are embedded in a ring of fullerene molecules with a constant width.

9:12AM H23.00007 Self-Assembly of Thiol Adsorbates on the Au(111)surface, FRANK HAGELBERG, QUINTON WILLIAMS, JIAN-GE ZHOU, Jackson State University — A long-standing controversy related to the dimer pattern formed by methanethiol (CH$_3$SH) and methylthiolate (CH$_3$S) on the Au(111) surface has been resolved using density functional theory within periodic boundary conditions. It is found that the 5 atoms of methanethiol adsorbates on the Au(111) surface form Van der Waals dimers. For methylthiolate, it is shown that no dimerization occurs at high coverage. At intermediate coverage, however, a Van der Waals dimer pattern emerges. The presence of defects in the Au(111) surface does not change this conclusion. Molecular dynamics simulation at high coverage demonstrates that the observed dialkyl disulfide species emerge during the desorption process, and thus are not attached to the surface. A meta-stable monomer pattern has been shown to be only marginally higher in adsorption energy than the dimer pattern.

9:24AM H23.00008 Chemical pressure and hidden one-dimensional behavior, ANDREA SACCHETTI, LEONARDO DEGIORGI, ETH Zurich, THIERRY GIAMARCHI, University Geneva, NANCY RU, IAN FISHER, Stanford University — We report on the first optical measurements of the rare-earth tri-telluride charge-density-wave systems. Our data, collected over an extremely broad spatial range, allow us to observe both the Drude component and the single-particle peak, ascribed to the contributions due to the free charge carriers and to the charge-density-wave gap excitation, respectively. The data analysis displays a diminishing impact of the charge-density-wave condensate on the electronic properties with decreasing lattice constant across the rare-earth series. We propose a possible mechanism describing this behavior and we suggest the presence of a one-dimensional character in these two-dimensional compounds. We also envisage that interactions and umklapp processes might play a relevant role in the formation of the charge-density-wave state in these compounds.
Fermi-liquid effects in the magnetization oscillations in quasi-two-dimensional conductors, ALEXANDER ZIMBOVSKY, Urals State Mining University, NATALYA ZIMBOVSKAYA, University of Puerto Rico at Humacao — In this work we present the results of theoretical analysis of the Haas-van Alphen oscillations in quasi-two-dimensional metals. We have been studying the effect of the Fermi-liquid correlation of charge carriers on the above oscillations. It was shown that at reasonably low temperatures and weak electron scattering the Fermi-liquid interactions may cause noticeable changes in both amplitude and shape of the oscillations even at realistically small values of the Fermi-liquid parameters. Also, we show that the Fermi-liquid interactions in the system of the charge carriers may cause magnetic instability of a quasi-two-dimensional metal near the peaks of quantum oscillations in the density electron of states at the Fermi surface, indicating the possibility for the diamagnetic phase transition within the relevant ranges of the applied magnetic fields. The obtained results are applicable to strongly anisotropic organic metals, and to other quasi-two-dimensional compounds.

Interface mobility from interface random walk, ZACHARY TRAUTT, MONEESH UMPANYU, Colorado School of Mines, ALAIN KARMA, Northeastern University — Computational studies aimed at extracting interface mobilities require driving forces orders of magnitude higher than those occurring experimentally. We present a computational methodology that extracts the absolute interface mobility in the zero driving force limit by monitoring the one-dimensional random walk of the mean interface position along the interface normal. The method exploits a fluctuation-dissipation relation similar to the Stokes-Einstein equation, which relates the diffusion coefficient of this Brownian-like random walk to the interface mobility. Atomic-scale simulations of grain boundaries in model crystalline systems validate the theoretical predictions, and also highlight the profound effect of impurities. The generality of this technique combined with its inherent spatial-temporal efficiency should allow computational studies to effectively complement experiments in understanding interface kinetics in diverse material systems.

Ab-initio investigations on electronic and lattice dynamical properties on intercalation of Cu (copper) into hexagonal boron nitride (hBN), BAHADIR ALTINTAS, Abant Izzet Baysal University, Dept. of Chemistry, CIHAN PARLAK, RESUL ERYIGIT, Abant Izzet Baysal University, Dept. of Physics, CETIN BOZKURT, Abant Izzet Baysal University, Dept. of Chemistry — Layered structure of hexagonal boron nitride (hBN) and its intercalation with transition metals have been the subject of many recent studies. In this work, we investigate the electronic structure and the lattice dynamical properties of copper intercalated hBN by using Density Functional Theory (DFT) with a plane-wave basis set for the electronic wave functions and periodic boundary conditions. The interaction between valance electrons, the nuclei and the core electrons is described by norm-conserving pseudopotentials. We report the result of calculations on lattice geometry, electronic and lattice dynamical properties of the compound. Possible effects of Cu-incorporation on the structure of hBN were determined from a consideration of minimizing the quantum mechanical total energy and forces. Intercalated Cu atom is found to prefer the position between B and N atoms of two layers. The signature of intercalated Cu states were determined from the calculated electronic local density of states. The phonon frequencies were computed at the center of the Brillouin zone and four Cu-related bands were found at 187, 560, 960, 1206 cm⁻¹ which can be measured by IR spectroscopy.

Current-Driven Phase Oscillation and Domain-Wall Propagation in WₓV₁₋ₓO₂ Nanobeams, ABRAM FALK, QIAN GU, JUNCHAO WU, LIAN OUYANG, HONGKUN PARK, Harvard University — We report the observation of a current-driven metal (M)-insulator (I) phase oscillation in two-terminal devices incorporating individual WₓV₁₋ₓO₂ nanobeams connected in parallel with a shunt capacitor. The phase oscillation frequency reaches above 5 MHz for ∼1-µm-long devices. The M-I phase oscillation coincides with the charging/discharging of the capacitor and occurs through the axial drift of a single M-I domain wall driven by Joule heating and the Peltier effect.

Coincidence Measurements of the Auger Cascade Process in MnO, Ag and Pd, R. SUNDRAMOORTHY, A.H. WEISS, University of Texas at Arlington, S.L. HULBERT, NSLS, Brookhaven National Lab, R.A. BARTYNSKI, Rutgers University — The Auger spectra associated with Auger cascade processes provides a probe of many-electron phenomena, the effects of screening and correlation in the intermediate and final many hole states. Here we present the first direct measurements of the energy spectra of electrons emitted in the later steps of Auger cascade processes in MnO, Pd and Ag performed using Auger-Auger coincidence spectroscopy (AACS). The Auger spectra resulting from the decay of core holes generated by a previous Auger cascade step (as measured by AACS) are shown to be broadened and shifted as compared to the Auger spectra resulting from the direct photo excitation of the corresponding core holes as measured by Auger photoelectron coincidence (APECs). The large differences between the Auger spectra resulting from the different origins of the core hole excitation are discussed in terms of the correlation effects in many hole excited states.

Scandium Oxide Thin Films and Their Optical Properties in the EUV, GUILLERMO ACOSTA, DAVID ALLRED, STEVE TURLEY, RICHARD VANFLEET, Brigham Young University — In recent years, it has been conjectured that scandium thin films could be used to produce highly reflective coatings in the Extreme Ultraviolet (EUV). However, scandium’s affinity to form new compounds prevents such coatings from achieving calculated reflectivities. In this project, thin films of scandium oxide are studied to supplement the understanding and use of scandium, and possibly as a substitute for scandium in multilayer coatings. This study reports on the physical and optical characterization of scandium oxide thin films. Thin films of scandium oxide, 15-50 nanometers thick, were deposited on silicon photodiodes by reactively sputtering scandium in an oxygen environment. These samples were measured using EUV synchrotron radiation at the Lawrence Berkeley National Laboratory Advanced Light Source, Beamline 6.3.2. Reflection and transmission measurements, at variable angles, were taken simultaneously from 2.7-50 nanometers. Analysis of the data has provided experimentally determined optical constants for scandium oxide thin films. The samples includes ellipsometry, scanning transmission electron microscopy, energy dispersive x-ray analysis, and high resolution transmission electron microscopy.

Quantum statistics for a finite number of polarons in a neutralizing background, FONS BROSENS, S.N. KLIMIN, J.T. DEVREESE, Universiteit Antwerpen — The ground state energy of an N-particle system, confined to a spherical quantum dot with a neutralizing background charge, is investigated within an all-coupling many-body path-integral variational principle, taking into account both the Fermi statistics of the polarons and the electron-electron interaction. The treatment of the ground-state energy is performed for both closed-shell and open-shell systems. The average fermion density in the neutral spherical dot is characterized by the Wigner-Seitz parameter r_s. For a sufficiently large but finite number of polarons, the dependency of the ground state energy on r_s is similar to that for a polaron gas in bulk. Herefrom, we can conclude that the ground state properties of a polaron gas in bulk can be qualitatively described using a model of a finite number of polarons in a confinement potential provided by a neutralizing background charge.

Tuesday, March 6, 2007 8:00AM - 10:36AM — Session H31 DCMP: Transport in Carbon Nanotubes: Theory — Colorado Convention Center 401
8:00AM H31.00001 First-principles studies of electrical transport in metal-contacted semiconducting carbon nanotubes, JUAN PALACIOS, Universidad de Alicante (Spain), P TARAKESHWAR, DAE KIM, KIAS (South Korea) — We present first-principles calculations of the transport properties of semiconducting carbon nanotubes (CNT’s), coupled to metallic electrodes. Our results indicate that, for realistic end-contact geometries, including atomic relaxation, the Fermi level position within the gap differs between palladium-contacted CNT’s and gold-contacted CNT’s. More interestingly, the contact resistance for the valence band in the case of Pd is much smaller than in the case of Au, while no significant difference is observed for the conduction band. This could explain experimental results showing that hole conduction is favored in the case of Pd contacts.

8:12AM H31.00002 First Principle Study of Electronic Transport in Carbon Nanotubes and Copper Nanowires for Interconnect Applications, YU ZHOU, YIMING ZHANG, SUBBALAKSHMI SREEKALA, PULICKEL AJAYAN, SAROJ NAYAK, DEPARTMENT OF PHYSICS, RPI TEAM — We will present our recent first principles calculation modeling work on carbon nanotubes (CNT) and copper wires for Interconnect applications. In particular we have calculated the ballistic transport properties of nanotubes based on their density of states and band structures, and compared with that of copper wires of similar dimension. By using Ohm’s law and Landauer Formalism, we computed the resistance of them in mesoscopic sizes. The effect of correlation in the transport properties are discussed in detail. We will present our work on the nanowires and nanotubes packing and their impact on the resistance, while taking into account the surface scattering based on Fuchs-Sondheimer model. The performance of CNT for both local and global Interconnects will be discussed in detail. Our results show that nanotube bundles can outperform copper wires for long intermediate and global interconnects.

8:24AM H31.00003 Interwall interactions and electrical conductance in telescoping carbon nanotubes, YONG-JIU KANG, Department of Physics, KAIST, YONG-HOON KIM, University of Seoul, KEE JOO CHANG, Department of Physics, KAIST — Telescopically aligned carbon nanotubes, where the inner core shells are pulled out from the house shells with larger diameters in multi-walled nanotubes, are good systems to interwall interactions and their effect on electron conduction. In several tight-binding calculations, there exists some controversy in the quantum conductance of telescoping nanotubes. In this work, using the non-equilibrium matrix Green function approach within the first principles local-density-functional approximation, we study the quantum transport behavior of the (5,5)/(10,10) telescoping nanotube. Varying the hybridized double wall region, we investigate the effect of interwall interactions on the electron transport and compare the results with those obtained from tight-binding calculations. Although individual tubes have two conducting channels at the Fermi level, only one channel gives rise to electrical conduction with antiresonance dips in transmission, while the other channel is suppressed. Thus, the maximum conductance is close to $G_0$, in contrast to single $\pi$-orbital tight-binding calculations, which showed the maximum conductance close to $2G_0$. Our first-principles calculations indicate that the tight-binding model significantly overestimates the interwall coupling between the inner and outer shells.

8:36AM H31.00004 Quantum transport in carbon nanotube field effect transistors, KALMAN VARGA, S.T. PANTELIDES, Vanderbilt University — We have investigated the transport properties of carbon nanotube field effect transistors using the recently developed source-and-sink method [1]. We report first-principles results on the current-voltage characteristics of semiconducting carbon nanotubes in transverse electric field, highlighting differences with Si-based devices, e.g., band mixing caused by the gate electric field. We also find that the source-drain current exhibits an intrinsic saturation as function of the gate voltage. The calculated results are in good overall agreement with pertinent experiments.


8:48AM H31.00005 Signature of the electron-electron interaction in the magnetic field dependence of the nonlinear I-V characteristics in non-centrosymmetric conductors, ERIC DEYO, BORIS SPIVAK, University of Washington, A. YU. ZYUZIN, A. F. Ioffe Institute — In non-centrosymmetric media, there exists a contribution to the nonlinear I-V characteristics which is linear in magnetic field and quadratic in voltage. This effect is entirely due to electron-electron interaction, and its magnitude is proportional to the electron-electron interaction constant. We present calculations of the magnitude of this effect in mesoscopic samples and in chiral carbon nanotubes as a function of temperature. In the case of a magnetic field oriented parallel to plane of a mesoscopic sample, the effect is proportional to both the electron-electron interaction constant and the spin-orbit scattering amplitude.

9:00AM H31.00006 Ab initio investigations of formation of the poly-bromine anions encapsulated inside the carbon nanotube, DONGCHUL SUNG, Sejong University, Seoul, Korea, NOEJUNG PARK, Dankook University, Seoul, Korea, SUKLYUN HONG, Sejong University, Seoul, Korea — We have performed ab initio density-functional calculations to investigate the electronic and geometric structure of the bromine adsorbates inside the carbon nanotube. It is found that the charged odd-membered molecular species (Br$_n$ or Br$_5$ ) are energetically favored inside the carbon nanotube rather than common Br$_2$ molecule. Vapor phase of bromine molecules (Br$_2$) could exothermically adsorb into the nanotubes, and in turn, transform into the Br$_3$ or Br$_5$ structures without a significant energy barrier. Such a formation of the poly-bromine anions accompanies a strong charge transfer from the nanotube to the adsorbates, rendering the encapsulating nanotube strongly hole-doped. We suggest that an exposure of the tip-opened carbon nanotube samples to a modest Br$_2$ partial pressure could result in strong hole-doped, and thus nearly metallic nanotube samples.

9:12AM H31.00007 Electron transport through molecular-carbon nanotube interfaces, NICOLAS BRUQUE, RAJEEV PANDEY, KHAIRUL ALAM, ROGER LAKE, UC Riverside — Investigations have focused on electron transport through metal-molecule systems. Less effort has been directed towards semiconductor-molecule systems, and the least attention has been given to electron transport through carbon nanotube-molecule systems. A specific implementation of the latter system consists of two CNT’s joined by a molecule, or a CNT-molecule-CNT system. Such a system can provide the electronic functionality of a resonant tunnel diode. The molecular contacts, i.e. the CNTs, are a $\sigma$-bond surface and, as such, they are both chemically and geometrically different from metal contacts or sp$^3$ semiconductor contacts. A model system is studied to focus solely on the interface geometry of two simple $\pi$-bond systems, CNTs and polyacetylene (CH)$_n$. The system is CNT-(CH)$_n$-CNT. At the interface, in the relaxed structure, the (CH)$_n$ is oriented coplanarily with the tangential plane of the CNT. The transmission, calculated with our DFT (FIREBALL)-NEGF code is, on average, 3 or more orders of magnitude larger than the transmission of an unrelaxed structure in which the (CH)$_n$ is perpendicular to the CNT at the point of contact. This is also true when the (CH)$_n$ of the relaxed structure undergoes a 180$^\circ$ twist. Interface geometry plays a crucial role in the electron transport.

9:24AM H31.00008 ABSTRACT HAS BEEN MOVED TO V31.00015 —
9:36AM H31.00009 Effects of Electron-phonon scattering on Conductance of Carbon nanotubes using Time-dependent wave-packet approach1, HIROYUKI ISHII, CREST-JST, NOBUHIKO KOBAYASHI, University of Tsukuba, KENJI HIROSE, NEC Corporation — The application of single-walled carbon nanotubes as the ideal ballistic conductors is expected. However, the electronic current saturates at the high-bias regime due to electron-phonon scattering. In order to improve the conductivity, understanding of the scattering mechanism is highly required. We investigated the electron-phonon coupling effect on the conductance in single-walled carbon nanotubes using the time-dependent wave-packet approach under a tight-binding approximation [1]. The vibrational atomic displacements in real space are introduced through the time-dependent change of the transfer energies. We solve the time-dependent Schrödinger equation and obtain the time-dependent diffusion coefficients of the electronic wave packets. From these data, we can extract the coherence length and then the conductance. We found that the optical phonon decreases the conductance of metallic carbon nanotubes, because the propagating speed of electron is reduced by the electron-phonon scattering. Furthermore, we clarify the difference of the scattering effects on the conductivity of the metallic nanotube and the semiconducting one. [1] S. Roche et al., PRL 95 (2005) 076803

3This work is supported by the CREST project.

9:48AM H31.00010 ABSTRACT WITHDRAWN —

10:00AM H31.00011 Model Calculation for Molecular Junctions in between Carbon Nanotube Leads.1, YIING-REI CHEN, National Taiwan Normal University, LEI ZHANG, MARK HYBERTSEN — We present analytical and numerical calculations for several prototypes of molecules in a CNT-molecule-CNT junction. The properties of the transmission function at the Fermi level reveal the influence from the CNT symmetry and the nature of the molecules. In particular, we discuss and compare both one-point contact and two-point contact cases, so as to illustrate how the Fermi level transmission of a multi-point junction can be either larger or smaller than that in the single-molecule case, depending on the choice of contact sites.

1NSF, NSC

10:12AM H31.00012 Quantum electron transport in toroidal carbon nanotubes with metallic leads. , MARK JACK, MARIO ENCINOSA, Florida A&M University, Department of Physics, Tallahassee, FL 32307. — Carbon nanotubes and carbon nanotori possess all the interesting new electronic features seen in graphene e.g. massless Dirac fermion characteristics, small spin-orbit coupling effects, and quantized conductance, along with interesting curvature and boundary condition effects closing the tube to form a torus. The authors calculate electronic transport properties such as density-of-states and transmissivity for toroidal carbon nanotubes with attached metallic or carbon nanotube leads as functions of the lead positions. A tight-binding Hamiltonian for the nanotorus is applied to a 24-carbon-atom armchair unit cell. The closure of the straight tube to a toroidal geometry introduces an additional off-diagonal coupling term, not encountered for the straight case. The device Green’s function is then evaluated in tight-binding approximation using a recursion method to systematically determine its diagonal and off-diagonal matrix elements. References: 1. M. Encinosa and M. Jack, Phys. Scr. 73 (2006) 439-442. 2. M. Encinosa and M. Jack, Excitation of surface dipole and solenoidal modes on toroidal structures. Photonics and Nanostructures (Elsevier), May 2006. (Submitted) 3. M. Encinosa and M. Jack, Dipole and solenoidal magnetic moments of electronic surface currents on toroidal nanostructures. J. of Computer-Aided Materials Design (Springer), May 2006. (In Press)

10:24AM H31.00013 Mechanical and electronic properties at the interface between the Si(100) surface and semiconducting carbon nanotubes , SALVADOR BARRAZA-LOPEZ, Virginia Tech — I discuss the ab initio mechanical and electronic properties of semiconducting carbon nanotubes adsorbed on the Si(100) surface. After revising results from nanotubes on the fully unpassivated surface[1], the interaction between a semiconducting nanotube and a fully H-passivated Si(100) surface with dopants is examined[2]. As silicon wafers are ordinarily doped, the model closely resembles experimental conditions[2,3,4], allowing for qualitative comparison. The single H-monolayer prevents electronic states in nanotubes from energetically shifting along with those of the doped supporting substrate, permitting the engineering of the relative positions of the slab and nanotube band edges. Finally, and following experimental work, we study adsorption characteristics of nanotubes on partially passivated surfaces. Surface states in the unpassivated regions modify the electronic structure of the interface and provide for the anchoring of nanotubes, deforming them in some cases. Results with and without dopants will be given[2].


Tuesday, March 6, 2007 8:00AM - 10:48AM –

Session H42 DCMP: Metals on Metals Colorado Convention Center 505

8:00AM H42.00001 Effects of shadowing and steering in oblique-incidence metal growth1, J.G. AMAR, Y. SHIM, V. BOROVIKOV, University of Toledo — The effects of oblique incidence on the surface morphology in metal (100) epitaxial growth are studied using a simplified model which includes shadowing but not the effects of short-range and long-range attraction of depositing atoms to the surface. Surprisingly, we find that many of the qualitative features observed in oblique incidence Cu(100) growth, including the existence of anisotropy in the submonolayer regime, as well as of a transition from anisotropic mounds to ripples perpendicular to the beam with increasing deposition angle, can be explained primarily by geometrical effects. We also find that the formation of (111) facets is crucial to the development of well-ordered ripples at large angles of incidence. A second transition from ripples oriented perpendicular to the beam to ‘rods’ with (111) facets oriented parallel to the beam is also found at very high deposition angles and film thicknesses. When the effects of short- and long-range interactions are included in our simulations, we find two main effects. In the submonolayer regime, attraction tends to weaken the effects of shadowing and reduce the submonolayer anisotropy. However, in the multilayer regime ‘flux-focusing’ due to long-range attraction tends to enhance the anisotropy and reduce the critical thickness/angle for the ripple transition. Near the transition from ripples to rods, sideways attraction also tends to stabilize the isotropic phase as is observed experimentally.

1Supported by ACS PRF and NSF
8:12AM H42.00002 Multiscale simulations of oblique-incidence Cu/Cu(100) epitaxial growth, M. Rajappan and C. P. Flynn, University of Illinois at Urbana-Champaign, MAHESH RAJAPPAN, Wellesley College, C. PETER FLYNN, University of Illinois at Urbana-Champaign, UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN TEAM — We present the results of multiscale simulations of oblique-incidence Cu/Cu(100) epitaxial multilayer growth carried out in order to explain the experimentally observed ripple formation at large deposition angles with respect to the substrate normal. Our method combines a kinetic Monte Carlo (KMC) simulation for the thermal surface diffusion with a small-scale one-atom molecular dynamics (MD) simulation of every deposition event, in order to account correctly for shadowing as well as the short-range and long-range attraction of depositing atoms to the surface. These simulations are particularly challenging both because of the existence of significant finite-size effects at large deposition angles, as well as because of the computational time required to simulate the deposition process, and therefore an efficient algorithm for carrying out parallel simulations of deposition will be described. The relative importance of shadowing and long-range attraction, as well as the dependence of the surface morphology on such parameters as the Ehrlich-Schwoebel barrier, edge- and corner-diffusion, and deposition flux will be discussed. Preliminary results in which both the substrate atoms and the depositing atom undergo molecular dynamics in the final stages of deposition will also be presented for comparison.

1Supported by ACS PRF and NSF

8:24AM H42.00003 Molecular Dynamics Simulations of Upward Diffusion of Adatoms and Clusters on Facetted fcc Metal (110) Surfaces, HAILI YANG, QIANG SUN, Zhengzhou University, Henan, China, SONGYOU WANG, Fudan University, Shanghai, China, SHUNFANG LI, Zhengzhou University, Zhengzhou, Henan, China, ZHENYU ZHANG, Oak Ridge National Laboratory, The University of Tennessee, YU JIA, Zhengzhou University, Zhengzhou, Henan, China — We study upward self-diffusion of adatoms and small clusters across the outer edges of the mounds formed in fcc metal(110) homoepitaxy using molecular dynamics simulations with interatomic potentials described by the embedded-atom method. Our results show that both single adatoms and small clusters on the (111) and (100) facets of Au and Cu(110) can readily diffuse upwards and cross the outer edge of the mounds, but with different atomistic mechanisms. An adatom crosses the outer edge via a simple place exchange or indirect exchange mechanism. In contrast, the upward diffusion and outer-edge crossing of small clusters is realized by their dissociation at the edge of the mound after one or two cluster atoms are incorporated into the edge. Our simulations reveal that there truly exists efficient upward mass transport in homoepitaxy on faceted fcc metal (110) surfaces.

1Supported by NSF of China, the BES program of US DOE, & USNSF

8:36AM H42.00004 Surface mass diffusion on Pt(111), MICHAL ONDREJCEK, WACEK SWIECH, University of Illinois at Urbana-Champaign, MAHESH RAJAPPAN, Wellesley College, C. PETER FLYNN, University of Illinois at Urbana-Champaign, UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN TEAM — We describe investigations of relaxing steps on Pt(111) in the temperature range 690-1250K. This extends the range over which surface mass diffusion coefficient D_s is known from step fluctuation spectroscopy (SFS) on Pt(111) [1]. A beam of Pt^− self-ions is used in situ to create quasi sinusoidal step structures on the surface. The beam with impact energy 1kV initially creates at elevated temperatures vacancy islands that merge with steps. The decay process of periodic features driven by the gradient in the chemical potential is observed by low energy electron microscopy (LEEM). The diffusion coefficients are evaluated from the relaxation times as a function of wave number q for Fourier components of the step edge displacements. The quantitative results of D_s are compared to the previously measured values at temperatures T>1200K [1]. The agreement in regime where data overlap is quite remarkable. Both sets of results yield values for the surface mass diffusion coefficient, D_s = 4 x 10^{-14} exp(-1.45 eV/k_B T) cm^2/s. [1] M. Ondrejcek, W. Swiech, M. Rajappan and C. P. Flynn, Phys.Rev.B 72 085422 (2005)

1This research is supported by DOE grant DEFG02-91-ER45439.

8:48AM H42.00005 Ab initio calculation of atomic interactions on Al(110): implications for epitaxial growth, KRISTEN FICHTHORN, YOGESH TIWARY, Penn State University — Using first-principles calculations based on density-functional theory, we resolved atomic interactions between adsorbed Al atoms on Al(110). Relevant pair and trio interactions were quantified. We find that pair interactions extend to the third in-channel and second cross-channel neighbor on the anisotropic (110) surface. Beyond these distances, pair interactions are negligible. The nearest-neighbor interaction in the in-channel direction is attractive, but nearest-neighbor cross-channel interaction is repulsive. While nearest-neighbor, cross-channel repulsion does not support the experimental observation of 3D hut formation in Al/Al(110) homoepitaxial growth [1], we find that trio interactions can be significant and attractive and they support cross-channel bonding. The pair and trio interactions have direct and indirect components. We have quantified the electronic and elastic components of the indirect, substrate-mediated interactions. We also probe the influence of these interactions on the energy barriers for adatom hopping. [1] F. Buatier de Mongeot, W. Zhu, A. Molle, R. Buzio, C. Boragno, U. Valbusa, E. Wang, and Z. Zhang, Phys. Rev. Lett. 91, 016102 (2003).

1Supported by NSF DMR 0514336

9:00AM H42.00006 Multi-scale simulation of quantum dot formation in Al/Al (110) homoepitaxy, YOGESH TIWARY, KRISTEN FICHTHORN, Penn State University — In experimental studies of Al(110) homoepitaxy, it is observed that over a certain temperature window (330-500K), 3D huts, up to 50 nm high with well defined and smooth (111) and (100) facets, form and self-organize on the micron scale [1]. The factors leading to this kinetic self-organization are currently unclear. To understand how these structures form and evolve, we simulated multi-layer, homoepitaxial growth on Al(110) using ab initio kinetic Monte Carlo (KMC). At high temperatures, where nano-huts form, the KMC simulations are slow. To tackle this problem, we use a technique developed by Devita & Sander [2], in which isolated adatoms make multiple moves in one step. We achieve high efficiency with this algorithm and we explore very high temperatures on large simulation lattices. We uncover a variety of interesting morphologies (Ripples, mounds, smooth surface, huts) that depend on the growth temperature. By varying the barriers for various rate processes, we discern the factors that determine hut sizes, aspect ratios, and self-organization. [1] F. Buatier de Mongeot, W. Zhu, A. Molle, R. Buzio, C. Boragno, U. Valbusa, E. Wang, and Z. Zhang, Phys. Rev. Lett. 91, 016102 (2003). [2] J.P. Devita & L.M. Sander, Phys. Rev. B 72, 205421 (2005).

1Supported by NSF DMR 0514336
9:12AM H42.00007 Positron trapping at quantum-dot like Cu nano-particles embedded in Fe and submonolayer films of Au and Pd deposited on Cu(100) surface. N. G. FAZLEE, A. H. WEISS, Physics Department, University of Texas, Arlington — Recently clear evidence has been provided that positron spectroscopy can be used to characterize the properties of quantum-dot-like nano-particles embedded in host material even at dilute levels as a result of the preferential trapping of positrons in the nano-particles. The results of studies of sputtered surfaces of the Fe-Cu alloy with quantum-dot like Cu nano-particles embedded in the top atomic layers of Fe and submonolayer films of Au and Pd deposited on Cu(100) using Positron-Annihilation-Induced Auger-Electron Spectroscopy are analyzed by performing calculations of positron surface states and annihilation characteristics. Estimates of the positron binding energy, work function and annihilation characteristics performed for studied surfaces reveal their sensitivity to nano-particle size and coverage. Trapping of positrons at nano-particles on studied surfaces is determined from calculated positron surface state wave functions and comparison of theoretical core annihilation probabilities with experimental ones estimated from the measured Auger peak intensities.

9:24AM H42.00008 Adatom Diffusion on Ag(100) and Cu (100) Surface with Steps: insights from ab initio electronic structure calculations JIEBING SUN, Department of Physics, University of New Hampshire, JAMES B. HANNON, IBM T. J. Watson Research Center, GARY L. KELLOGG, Sandia Corporation, a Lockheed Martin Company, for the U.S. DOE's NNSA under Contract DE-AC04-94AL85000. The results of measurements of Pd films on Cu(001) have been experimentally determined using low energy electron microscopy (LEEM). We describe Monte Carlo simulations that show that the Pd distribution in the 3rd layer is heterogeneous due to step overgrowth during Pd deposition. Interestingly, the Pd distribution in the 2nd layer is also heterogeneous, and appears to correlate with the distribution in the 1st layer. We describe Monte Carlo simulations that show how to deal with this phenomenon using a quarto interactions. We comment on extensions to (110) faces and analytic expressions for step stiffness.

9:36AM H42.00009 Quantum Size Effect on Adatom Surface Diffusion JINFENG JIA, Department of Physics, Tsinghua University, Beijing 100084, China, LIYING MA, LIN TANG, XUCUN MA, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China, QIKUN XUE, Department of Physics, Tsinghua University, Beijing 100084, China; Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China, Y. HAN, STEVE HUANG, FENG LIU, Department of Material Science and Engineering, University of Utah, Salt Lake City, Utah 84112 — Using scanning tunnelling microscopy, we demonstrate the nucleation density of Fe islands on surface of nanoscale Pb films oscillates with film thickness, providing a direct demonstration of quantum size effect on surface diffusion. The Fe adatom diffusion barriers were derived to be 204 and 187 meV on a 21 and 26 monolayer (ML) Pb film, respectively, by matching the kinetic Monte Carlo simulations to the experimental island densities. The effect is further illustrated by growth on wedged Pb films, where the Fe island density is consistently higher on the odd-layer films than on the even-layer films in the thickness range of 11 to 15 ML.

9:48AM H42.00010 Multisite Adatom Relaxations in Lattice-Gas Models of Adsorbates: Reconciling Adatom Relaxations at Steps T.L. EINSTEIN, RAJESH SATHIYANARAYANAN, T.J. STASEVICH, U. of Maryland — In a lattice-gas (LG) framework for (111) cubic surfaces, pair interactions cannot distinguish A and B steps, but an orientation-dependent three adatom (trio) interaction can, as we verify with VASP for Cu(111). However, on Pt(111), small clusters considerably underestimate the difference. For a sequence of overlayer configurations, we explore the role of lateral relaxations and how they complicate LG analysis. On Cu(100) our prior VASP calculations of a particular trio interaction energy (E_t) nearly cancels the attractive second-neighbor interaction energy (E_2), leading to a discrepancy between theory and experiment of step stiffness anisotropy. Relaxations at step edges greatly reduce this repulsion. Since position-dependent interactions are improper in LG models, we show how to deal with this phenomenon using a quarto interactions. We comment on extensions to (110) faces and analytic expressions for step stiffness.
Tuesday, March 6, 2007 11:15AM - 2:15PM – Session J1 DCMP: Cuprate Superconductors: Underdoping and Pseudogaps

11:15AM J1.00001 Nernst effect, fluctuation diamagnetism and vortices above Tc in cuprates

N. PHUAN ONG, Princeton University — Nernst-effect and torque magnetometry experiments have provided evidence that, in the hole-doped cuprates, long-range phase coherence vanishes at the critical temperature \( T_c \), while the pair condensate survives to a much higher “onset” temperature \( T_{\text{onset}} \). In the Nernst experiment, the vortex current produced by a gradient generates a Josephson \( E \)-field perpendicular to the applied field \( H \). In cuprates, this large Nernst signal \( E_N \) persists to \( T_{\text{onset}} \sim 130 \) K. Extensive Nernst experiments in the cuprates LSCO, Bi 2201, and 2212 yield a 3D phase diagram \((x, T, H)\) in fields up to 45 T. This picture has been confirmed by high-resolution torque magnetometry. In a tilted \( H \), local planar supercurrents associated with vortices above \( T_c \) produce a torque that deflects a cantilever. At each \( T_c \), the diamagnetic magnetization inferred matches the field profile of the Nernst \( E_N \). The high-resolution measurement of the diamagnetic susceptibility \( \chi \) over 5 field decades uncovers an unusual, fragile “London rigidity” that exists in the pseudogap state of Bi 2212 and 2201. The magnetization curves below \( T_c \) also provide a reliable determination of the upper critical field \( H_{c2} \) which is found to scale linearly with \( T_{\text{onset}} \). I will also present evidence for pairing without phase coherence at 0.35 K in LSCO for \( x < x_c \) in fields to 30-45 T. In collaboration with Yayu Wang, Lu Li, Joseph G. Checkelsky, Michael Naughton, Seiki Komiya, Shimpei Ono, Yoichi Ando, Shin-ichi Uchida and Genda Gu.

11:51AM J1.00002 Controversial Issues in High-\( T_c \) Superconductivity - a Specific Heat Perspective

JOHN LORAM, Cambridge University, UK — We briefly review specific heat data on the evolution with hole doping of HTS cuprates and discuss the results in terms of current models. We see a universal progression from insulator to overdoped metal via a states-non-conserving approximately \( V \)-shaped pseudogap in the \( qp \) DOS. The gap shrinks with \( \rho \) due to the accumulation of new spectral weight (~ 1 state per doped hole) on the shoulders of the pseudogap (the antinodal regions) and closes abruptly close to optimal doping accompanied by a rapid increase in superconducting (SC) condensation energy. Thermodynamic measurements show no features (even broadened) at the temperature \( T* \) at which the pseudogap is generally presumed to close, and that the spectral weight loss persists to temperatures well above \( T* \). This suggests that the pseudogap is not due to a Fermi surface instability or precursor SC fluctuations and that the pristine Fermi surface is not restored at \( T* \). Specific heat and NMR measurements also reveal a rather high degree of SC homogeneity, casting doubt on the popular inference of gross SC gap inhomogeneity revealed by some tunnelling studies.

12:27PM J1.00003 From Fermi Arcs to the Nodal Metal

MICHAEL NORMAN, Materials Science Division, Argonne National Laboratory — The pseudogap phase in the copper oxide superconductors is a most unusual state of matter, and understanding its nature will likely resolve the issue of what interactions give rise to the superconductivity itself. Angle resolved photoemission has revealed that the pseudogap phase is characterized by a partially truncated Fermi surface, denoted as a Fermi arc. We have found that the arc length is proportional to \( T/\Delta^* \), where \( \Delta^* \) is the pseudogap temperature. Therefore, in the zero temperature limit, the pseudogap phase has the same nodal structure as the d-wave superconducting phase. Attempts to explain this novel behavior by a variety of theoretical models will be discussed, as well as the fate of these Fermi arcs once superconductivity sets in.

1Supported by NSF-CAREER-DMR-0134933 and ACS-PRF-37999-G5

2Resarch supported by NSF DMR 0213706.
We close by proposing directions for future work. We compare with experimental data from polyfluorenes. We discuss ways in which low-T universal transport can break down, and in particular focus on the importance of strong correlations, which can reduce local coherence in the presence of disorder or other spatial perturbations. Static magnetism coexisting with superconductivity has been detected in some but not all cuprate families, particularly at low temperatures and for strongly underdoped systems. We present an interpretation of this superconducting “spin glass” state as local antiferromagnetic order driven by dopant atoms, particularly in the LSCO and BSCCO systems. Within this framework, recent NMR experiments on Zn-doped YBCO can also be quantitatively explained, down to detailed description of the lineshapes. Both the strong correlations and the quantum interference of impurity states appear to be vital to understand these results. In either more disordered or more underdoped systems, the tendency towards static magnetism is enhanced. Numerical solutions of the Bogoliubov-de Gennes equations of a disordered d-wave superconductor with Hubbard-like correlations show that in this case $\kappa_0$ is in fact strongly suppressed, universality of quasiparticle transport is violated and $\kappa_0$ may no longer be used to extract the size of the gap near the node directly.

1 Supported in part by DOE DE-FG02-05ER46236.

2 B.M. Andersen and P.J. Hirschfeld, cond-mat/0607082, J.W. Harter et al., cond-mat/0609721

3Supported by DOE through BES and LDRD at Los Alamos.

1:39PM J3.00005 Cross-Cutting Basic Research Needs for Solid State Lighting\(^1\), JAMES MISEWICH, Brookhaven National Lab — The recent DOE workshop on basic research needs for solid-state lighting has identified a number of cross-cutting scientific research areas that have potential to impact solid-state lighting. Basic research in the following areas were identified as priorities: new functionality through heterogeneous nanostructures, innovative photon management, enhanced light-matter interactions, multiscale modeling for solid-state lighting, and precise nanoscale characterization. We will provide an overview of the challenges and opportunities in these areas and describe how advances here could impact solid-state lighting.

\(^1\)This work was supported by the DOE Office of Basic Energy Sciences

Tuesday, March 6, 2007 11:15AM - 2:15PM – Session J10 DCMP: Superconductivity: Vortex Imaging Colorado Convention Center Korbel 1E

11:15AM J10.00001 Low Temperature STM Study of Vortex Motion on Fe doped NbSe2, HUI WANG, JONGHEE LEE, MICHAEL DREYER, Department of Physics, University of Maryland, College Park, MD 20742, BARRY BARKER, Laboratory for Physical Sciences, National Security Agency, 8050 Greenmead Drive, College Park, MD 20740 — We investigated the vortex motion around magnetic Fe impurities on type II superconductor NbSe2 by a home built low temperature STM. Using Scanning Tunneling Spectroscopy Maps we recorded the movie of the motion at 4 K with a very slow decaying rate of the magnetic field (\(\sim 5 \text{ nT/s}\)). The map images were taken with a 400 nm by 400 nm field of view and in a 0.75 T magnetic field to start with. Each frame of the movie has \(\sim 109\) vortices and takes \(\sim 8\) min to acquire. Scanning tunneling spectroscopy data show that the superconductivity is destroyed at the impurity sites, which indicates that they serve as attractive pinning centers for the vortex lattice. The behavior of the overall motion of the vortex lattice can be explained by the Larkin-Ovchinnikov collective pinning theory. The average speed of the motion is \(5 \text{ pm/s}\). Our STS movie data display the pinning and depinning events of a single vortex around the pinning center. A flux creep model will be exploited to understand the effect of the pinning centers on the vortex motion.

11:27AM J10.00002 Local vortex–defect interaction in moving vortex lattices observed by STM, MICHAEL DREYER, JONGHEE LEE, HUI WANG, University of Maryland, College Park, MD 20740, USA — When applying a magnetic field to a type II superconductor, part of the magnetic flux penetrates the sample forming a current vortex. At high enough fields and low enough defect concentration the vortices form a 2D triangular lattice. We observed the vortex lattice on NbSe\(_2\) single crystals using STM (\(B = 250 \text{ -- } 750\) mT, \(T = 4.2\) K). Due to a slow decay of the magnetic field of our superconducting magnet (\(\sim 5\) nT/s) the vortices collectively move at an average speed of about 5 pm/s. The motion was observed by tracking the center of a vortex across consecutive images of the vortex lattice. The motion shows distinct acceleration/deceleration cycles we associate with collective pinning events on nearby defect sites. A more subtle observation was the deviation of the vortex positions from their ‘expected’ location within the lattice of up to 3 nm. A similar effect was found in 2D simulations of a moving vortex lattice near defect sites. Since it takes an additional force to move a vortex out of position, we can identify subsurface defects and analyze the defect–vortex interaction. Results of the analysis will be presented.

11:39AM J10.00003 Lorentz Imaging of Superconducting Flux Vortices with a Commercial Transmission Electron Microscope\(^1\), JAMES LOUDON, PAUL MIDGLEY, University of Cambridge — Magnetic flux penetrates type II superconductors along normal channels called flux vortices, each containing a single quantum of flux. It is beneficial to image these vortices and study their response to external stimuli as they determine the performance of many superconducting devices. Tonomura’s research group have demonstrated that vortices can be imaged by transmission electron microscopy because of the deflection the electrons suffer as they pass through the magnetic flux within the vortices (Harada K. et al., Nature 360, 51, 1992). This technique offers spatial resolution superior to other techniques, real-time imaging and is sensitive to magnetic flux throughout the material, not simply surface fields. To our knowledge, Tonomura’s is the only group to have successfully employed this technique and their experiments required custom-built high voltage microscopes. Here we demonstrate that flux vortices can be imaged with a commercially available electron microscope, opening the field for other researchers. We show images of flux vortices in Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\), and analyze their arrangements as a function of applied magnetic field and temperature.

\(^1\)This work was funded by EPSRC, UK; Homerton College, University of Cambridge and Cornell Center for Materials Research, NSF-MRSEC

11:51AM J10.00004 Single Vortex Resolution Imaging of the Flux Front in a YBa\(_2\)Cu\(_3\)O\(_7-\delta\) Single Crystal, LAN LUAN, O. M. AUSLAENDER, K. A. MOLER, Stanford University, D. A. BONN, RUIXING LIANG, W. N. HARDY, University of British Columbia — We have imaged the vortex state in an optimally doped, detwinned YBa\(_2\)Cu\(_3\)O\(_7-\delta\) single crystal, using magnetic force microscopy (MFM). The structure of the flux front, the boundary between vortices and anti-vortices, is studied with single vortex resolution, as it evolves with applied magnetic field. We find the front to be corrugated on a scale of several microns. On a smaller scale, the front is composed of alternating “fingers” of vortices and anti-vortices. We also observe stable vortex-antivortex pairs.

12:03PM J10.00005 Magnetic Induction Profile in Superconductor/Ferromagnet Bilayers, QIANG LI, ZUXIN YE, Brookhaven National Laboratory — Strong suppression of flux density peaks at the edge of a superconducting film was observed by magnetooptical imaging of the magnetic induction profiles of an YBCO superconducting film on a magnetic substrate in perpendicular magnetic fields. The observed induction profile is in a striking contrast to the case of superconducting films on a non-magnetic substrate that display sharp flux density peaks at the edges of the films. The influence of magnetic substrate on the flux distribution in superconductor films may be modeled by considering the formation of a virtual infinite stack of superconducting films due to the magnetic mirror effect. We also found that the flux patterns in the magnetic substrate were strongly influenced by the flux distribution in the superconductor. These observations, results of computer simulations, and their implications to the transport and magnetization properties of superconducting films will be discussed.

12:15PM J10.00006 Dragging Individual Vortices to Probe the Dimensionality of Pinning in YBa\(_2\)Cu\(_3\)O\(_7-\delta\), O. M. AUSLAENDER, LAN LUAN, K. A. MOLER, Stanford University, R. A. HUGHES, J. S. PRESTON, McMaster University, D. A. BONN, RUIXING LIANG, W. N. HARDY, University of British Columbia — We have used a magnetic force microscope (MFM) to image and to manipulate individual vortices in optimally doped YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) samples: a 200nm film and a detwinned single crystal. In the film, if the force exerted by the MFM tip is strong enough to overcome the pinning potential, a pinned vortex jumps as a whole to a new pinning site. We find a wide spread of depinning forces, attesting to the importance of point pinners as opposed to pinning along one-dimensional defects. The behavior in the single crystal is very different. Even when a vortex is pinned the shape of its image is distorted, perhaps indicating meandering of the vortex line to take advantage of pinning centers as it traverses the crystal. When we drag a vortex, it tills significantly before depinning, as signified by pronounced stretching of its image. This effect is highly anisotropic and depends on the pulling direction.
12:27PM J10.00007 Manipulation of the magnetic flux in superconductor by the ferromagnetic domains in SC/FM hybrid, VITALII VLASKO-VLASOV, ULRICH WELP, GORAN KARAPETROV, VALENTIN NOVOSAD, Argonne National Laboratory, ANDREI BELKIN, Argonne National Laboratory & Illinois Institute of Technology, DANIEL ROSENMANN, WAI KWOK, Argonne National Laboratory — We studied magneto-optically the magnetic flux entry and exit in SC/FM hybrid of a ferromagnetic permalloy film sputtered on the superconducting NbSe2 single crystal. The FM film had growth induced perpendicular anisotropy and the labyrinth equilibrium domain structure. However, we could align the domain walls in a desired direction by application of a strong enough in-plane field. Thus formed stripe domains introduce a pronounced directionality for the vortex motion in the underlying superconductor. The effect persists up to the fields of the stripe domain collapse and does not depend on the temperature at which the domain walls were polarized. It does not change at heating the sample and cooling back below Tc.

We discuss the effect in terms of the domain wall pinning of vortices in conditions when the domain size is larger than the coherence length and propose a scheme for manipulating the transport properties of superconductors by the ferromagnetic domains.

1This work was supported by DOE, BES-Materials-Sciences under Contract DE-AC02-06CH11357

12:39PM J10.00008 Magnetic Force Microscopy of Superconducting Vortices in an Ordered Array of Artificial Pinning Centers, JOEL KEAY, PRESTON LARSON, KEVIN HOBBS, MATTHEW JOHNSON, Dept. of Physics and Astronomy, University of Oklahoma, Norman, OK 73019, OPHIR AUSLAENDER, KATHRYN MOLER, Stanford University, JOHN KIRTLEY, IBM Research Division, Yorktown Heights — Ordered arrays of artificial pinning centers were fabricated in Nb thin films using anodic aluminum oxide (AAO) as a template. These artificial pinning arrays have a triangular lattice parameter of 105 nm and antidot diameters of about 50 nm. The nanohole arrays show only a small decrease in the superconducting transition temperature, Tc=7.1 K, from comparable unprocessed Nb thin films. Enhancement of the magnetization at the first, second and third matching fields (matching field = 2170 Oe) were observed in the magnetization half-loops of these arrays at 5 K. Magnetic Force Microscopy (MFM) was used to image the nanohole arrays above and below Tc. These images clearly show the nanohole lattice. Individual vortices have been imaged at low fields and their movement within the lattice is being explored. Further, domain rings have been imaged at low and high fields at temperatures between 5 and 5.5 K. Their properties are currently being investigated.

1This work was supported by NSF grant nos. DMR-0080054 and NSF-0132534.

12:51PM J10.00009 Vortex dynamics in mesoscopic weak-pinning superconducting channels with a Corbino geometry, T.W. HEITMANN, K. YU, C. SONG, B.L.T. PLOURDE, Syracuse University, M.B.S. HESSELBERTH, P.H. KES, Leiden University — We report transport measurements of vortex flow dynamics in mesoscopic weak-pinning channels of a-NbGe with strong-pinning NbN channel edges. The channels are arranged in circular patterns on a Corbino disk geometry, thus eliminating the influence of edge barriers to vortex entry on the dynamics. The number of vortices which can be detected at particular flow velocities is limited by the method for measuring the flux flow voltage and the channel configuration. We discuss potential applications of this system for guiding vortices around nanofabricated structures free from edge barriers.

Supported by NSF DMR-0547147.

1:03PM J10.00010 Structured pinning potentials for guiding vortex motion in superconductors, K. YU, T.W. HEITMANN, C. SONG, B.L.T. PLOURDE, Syracuse University, M.B.S. HESSELBERTH, P.H. KES, Leiden University — Nanofabricated pinning structures can be used to guide vortices in superconductors through various potential energy landscapes. We report transport measurements of vortex flow dynamics in structured weak-pinning channels of a-NbGe with strong-pinning NbN channel edges. By arranging the channels in circular patterns on a Corbino disk geometry, we eliminate the influence of edge barriers to vortex entry on the dynamics. Patterning channel edges with different shapes allows us to explore the influence of the confinement potential on the vortex dynamics. We discuss one such pattern with channel edges in an asymmetric sawtooth configuration for investigations of vortex ratchet dynamics.

Supported by NSF DMR-0547147.

1:15PM J10.00011 Dynamic flux-quantum phases in weak-pinning V3Si and Re3W, A. A. GAPUD, J. D. HEBERT, A. MORADMAND, P. SHRESTHA, A. KHAN, U. of South Alabama, Y. ZUEV, D. K. CHRISTEN, Oak Ridge National Laboratory, V. KUZNETSOVA, J. R. THOMPSON, U. of Tennessee — The dynamics of transport-driven flux quanta in the absence of pinning is a fundamental phenomenon little understood and studied by few. This is mainly because of a rarity of highly homogeneous type II samples with few pinning defects, combined with the technical challenge of passing high levels of transport current through such samples. These issues are addressed by the use of ultrasonically soldered leads and pulsed currents, in addition to the availability of relatively defect-free samples of the low-temperature superconductors, V3Si and Re3W. This enabled the study of the critical-current “peak effect” in V3Si [PRB 67, 104516], which also included the observation of metastable phases in connection with the peak effect, still to be reported in greater detail. Another observation is that of dissipative flux flow phases, in both V3Si and Re3W, along with evidence of an approach towards the highly-ordered Bardeen-Stephen phase of free flux flow. The field dependence of free flux flow resistivity is also of interest in probing vortex core size effects [PRB 71, 134505]. All of these are to be discussed in detail. Research at ORNL supported by DOE Office of Electricity Delivery and Energy Efficiency and DOE Office of Science, Basic Energy Sciences.

1:27PM J10.00012 Vortex-antivortex molecules in superconducting films with magnetic dot arrays, M.V. MILOSEVIC, J.S. NEAL, S.J. BENDING, Department of Physics, University of Bath, BA2 7AY, UK, A. POTENZA, C.H. MARROWS, School of Physics and Astronomy, University of Leeds, LS2 9JT, UK — Following earlier works [Milosevic and Peeters, PRB (2003), PRL (2004)], we studied the vortex-antivortex stabilization in a superconducting film under a square array of magnetic dots of variable size. The theoretical side of the investigation was done within the Ginzburg-Landau theory, and main findings comprise: (i) multi-shell vortex-antivortex structures, (ii) the profound interaction between neighboring vortex-antivortex molecules through exchange of “valence” antivortices, and (iii) dual interaction of stabilized vortex-antivortex pairs and magnetic dots with excess flux-lines of the applied homogeneous magnetic field. On experimental side, the results are corroborated by scanning Hall probe measurements, performed on a 80nm thick Pb film, on top of a square array (period sum) of magnetic dots of four sizes - R=0.522, 0.738, 0.808, and 0.902/µm, etched out of a [2nm Pt] [0.6nm Co/1.0nm Pt]10 multilayer film with perpendicular magnetization. A 20nm thick Ge layer was evaporated on top of the dots to avoid the proximity effect. In measurements performed at T=5K, direct SHPM images showed the structure of antivortices between the magnetic dots, whereas the successive difference images revealed the positioning of additional vortices in applied homogeneous magnetic field.
1.39PM J10.00013 Vortex-antivortex phenomena in superconductors with antidot arrays. GOLIB-JON BERDIYOROV, MILORAD MILOSEVIC, ROELAND GEURTS, FRANCOIS PEETERS, Departement Fysica, Universiteit Antwerpen (CGB), Belgium — We investigated in detail the vortex configurations in superconducting films with regular antidot-arrays within the non-linear Ginzburg-Landau theory, where demagnetization effects and overlapping vortex cores are fully taken into account (contrary to the London approach). In addition to the well-known matching phenomena, we predict: (i) the nucleation of giant-vortex states at interstitial sites; (ii) the combination of giant- and multi-vortices at rational matching fields; and (iii) for particular interstitial vorticity, the symmetry imposed creation of vortex-antivortex configurations. As a consequence of (iii), we predict resistance maxima at particular matching fields, opposite to the expected minima due to commensurability effects. Using the same principle, we stabilized vortex-antivortex molecules in finite submicron superconducting polymers by strategically placed nanoholes. Compared to earlier predictions, we enhanced the stamina of the antivortex with respect to temperature, applied fields and geometrical defects in the sample. Further, increased vortex-antivortex spacing and pronounced amplitudes of the local magnetic field in our system make these fascinating structures observable by e.g. Scanning Tunneling or Hall probe microscopy.

1.51PM J10.00014 Novel Commensurability Effects and Enhanced Pinning at Nonmatching Fields for Vortices Interacting with Diluted Periodic Pinning Arrays. CHARLES REICHARDT, CYNTHIA J. OLSON REICHHARDT, Theoretical Division, Los Alamos National Laboratory — Using numerical simulations, we demonstrate that periodic pinning arrays that have been diluted by removing some fraction of the pinning sites often have commensurability effects at the same field strength as undiluted pinning arrays. The commensuration can occur at fields significantly higher than the field corresponding to one-to-one matching between the diluted pinning array and the vortices, and the effect persists for periodic arrays with up to 90 percent dilution. We show that samples with diluted periodic pinning arrays produce a considerable enhancement of the critical current for fields above the first matching field compared to samples with purely random pinning arrangements. These results suggest that diluted periodic pinning arrays may be a promising geometry to increase the critical current in superconductors over a wide magnetic field range.

2:03PM J10.00015 Influence of Au layer on the morphology and superconductivity of the ultra-thin Pb film using Low-temperature STM/S. SHENGYONG QIN, ALEXANDER KHAJEETOORIANS, CHIH-KANG SHIH, University of Texas at Austin — Thin film superconductivity is a subject of great scientific importance. Recently by using epitaxial thin Pb films, two papers reported the observation of quantum oscillations of thickness-dependent superconductivity. By using ex situ transport measurements on Pb thin films grown on Si(111) substrate and subsequently covered with 2 ML of Au, Guo et al. reported Tc oscillation between 22 and 28 MLs and a rapid decrease of Tc below 20 ML. On the other hand, Eom et al., by using in situ tunneling spectroscopy to measure the superconducting gap directly, reported persistent quantum oscillations of superconductivity from 18 ML down to 5 ML without any sign of quenching. One explanation of such apparent inconsistency is the existence of the Au capping layer used in the ex-situ transport measurements. Here we explore the role of Au capping layer on superconductivity of Pb thin film directly using STM/S. We show how the Au capping layer can induce significant roughening of the thin Pb film. Moreover, we found that the deposition of Au first induces the formation of AuPb alloy followed by Au overlay. Direct measurement of superconducting gaps on the film at different stages of Au deposition are also performed. The details of how Au overlay impact the superconductivity of thin Pb films will be presented.

Tuesday, March 6, 2007 11:15AM - 2:15PM — Session J23 DCMP: Metals: Actinides and Transport Colorado Convention Center 110

11:15AM J23.00001 Evolving Magnetism from self-damage in PuAm alloys. S.K. MCCALL, M.J. FLUSS, B.W. CHUNG, M.W. MCCLEFFRESH, G.F. CHAPLINE, Lawrence Livermore National Laboratory, R.G. HAIRE, Oak Ridge National Laboratory — As a consequence of the unusual nature of plutonium’s electronic structure, point- and extended-defects exhibit extraordinary properties. Low temperature magnetic susceptibility measurements on Pu and PuAm show that the magnetic susceptibility increases as a function of time, yet upon annealing the specimen returns to its initial value. This excess magnetic susceptibility rises from the α-decay and U recoil damage cascades which produce vacancy and interstitials as point and extended defects and at temperatures exceeds 10% of the annealed value after about 1 month of damage accumulation. Isochronal annealing measurements of α-Pu and stabilized δ-Pu reveal that the damage is frozen in place below ~30K and completely annealed away above 300K. The binary PuAm alloy follows a similar trend, but after warming to temperatures between 35 and 50K where defects are expected to begin moving, an enormous Curie like magnetic susceptibility arises with a Curie constant approximating 1 µemu/mole. This large magnetic susceptibility is significant, but after warming to temperatures above 50K the magnetic susceptibility disappears after 60K as further annealing takes place. Work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

11:27AM J23.00002 Study of Phonons in δ-Plutonium near the δ—α' Structural Phase Transition by X-ray Thermal Diffuse Scattering. RUQING XU, Univ. of Illinois at Urbana-Champaign, JOE WONG, Lawrence Livermore National Lab, PAUL ZSCHACK, Argonne National Lab, HAWOONG HONG, TAI-CHANG CHIANG, Univ. of Illinois at Urbana-Champaign — The 5f electrons in Pu can be either bonding or localized, depending sensitively on the temperature, pressure, and impurity doping. As a result, Pu displays a rich phase diagram involving a large number of phases of plutonium’s electronic structure, point- and extended-defects exhibit extraordinary properties. Low temperature magnetic susceptibility measurements on Pu and PuAm show that the magnetic susceptibility increases as a function of time, yet upon annealing the specimen returns to its initial value. This excess magnetic susceptibility rises from the α-decay and U recoil damage cascades which produce vacancy and interstitials as point and extended defects and at temperatures exceeds 10% of the annealed value after about 1 month of damage accumulation. Isochronal annealing measurements of α-Pu and stabilized δ-Pu reveal that the damage is frozen in place below ~30K and completely annealed away above 300K. The binary PuAm alloy follows a similar trend, but after warming to temperatures between 35 and 50K where defects are expected to begin moving, an enormous Curie like magnetic susceptibility arises with a Curie constant approximating 1 µemu/mole. This large effective moment disappears after 60K as further annealing takes place. Work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

11:39AM J23.00003 Lattice dynamics of the light actinides. JOHANN BOUCHET, CEA — Despite general interest in 5f-electron elements, details about their phonon-dispersion relationships are very limited. But recently, a new hope has emerged with several works, using inelastic x-ray scattering, mostly on U and Pu. Nevertheless all this experimental issues show that theoretical works are needed to tackle the 5f electrons systems. The lattice dynamics of the light actinides are known for almost 30 years, but until now any theory has been able to successfully reproduce these experimental data. Here we present the first ab-initio phonon spectrum of α-U[1]. We compare our spectrum obtained at 0 K with the neutron-scattering data obtained at room temperature with a particular attention to its anomalies. Then we predict the behavior of lattice dynamics of uranium as a function of pressure. We have also calculated the phonon spectra and the thermodynamic properties of Th, as the linear thermal expansion or specific heats[2], and the elastic properties of Th, Pa and U. [1]J. Bouchet submitted to Phys. Rev. Letter. [2]J. Bouchet, F. Jollet and G. Zerah, Phys. Rev. B 74 064637.
11:51 AM J23.00004 Density-Functional Calculations of \(\alpha\)-Pu-Ga (Al) Alloys, ALEXANDER LANDA, PER SODERLUND, Lawrence Livermore National Laboratory, Livermore, CA 94550, LEVENTE VITOS, Royal Institute of Technology, Stockholm, SE-10044, Sweden — At atmospheric pressure plutonium metal exhibits six crystal structures. The least dense phase (\(\delta\)-Pu) has a 25% larger volume than the ground-state (\(\alpha\)-Pu) phase and is thermodynamically stable at temperatures between 593 and 736 K. In order to extend the stability of \(\delta\)-Pu to ambient temperatures, plutonium is alloyed with a small amount of so-called \(\delta\)-stabilizers, for example, Ga or Al. The \(\alpha\)-phase has no equilibrium solubility with any of these \(\delta\)-stabilizers but upon cooling of the \(\delta\)-Pu-Ga (Al) alloys, under certain conditions, Ga (Al) atoms can be trapped in the \(\alpha\)-lattice causing an expansion. First-principles methods are employed to study the ground-state atomic volumes of \(\alpha\)-Pu-Ga (Al) alloys. It was shown that a random distribution of Ga (Al) atoms in the monoclinic lattice of \(\alpha\)-Pu results in a maximum expansion of this lattice. Any kind of ordering of Ga (Al) on the monoclinic lattice results in shrinking of the lattice constant while the ordered \(\alpha_{\delta}\)-Pu-Ga (Al)) configuration yields the smallest lattice constant which is very close to that of pure \(\alpha\)-Pu. In addition, energetics of the ordered and disordered configurations is discussed. This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

12:03PM J23.00005 The Elastic Moduli of Monoclinic and Orthorhombic Plutonium, ALBERT MIGLIORI, JON B. BETTS, C. PANTEA, I. MIHUT, C. MIELKE, J.N. MITCHELL, Los Alamos National Laboratory, LOS ALAMOS NATIONAL LABORATORY COLLABORATION — Measurements were made of the bulk and shear moduli of high-purity polycrystalline Pu from 10K to 670K using resonant ultrasound spectroscopy. A simple dilatometer was employed to provide redundant detection of the phase transitions. We observed the expected phase transitions from monoclinic (\(\alpha\)) to body centered monoclinic (\(\delta\)) to orthorhombic (\(\gamma\)) to face centered cubic (\(\delta\)). Very accurate values were obtained for \(\alpha\)-Pu, \(\beta\)-Pu was very soft and difficult to analyze, as was \(\delta\)-Pu. Surprisingly, the \(\gamma\)-phase produced the high-Q resonances needed for accurate elastic modulus determination. We discuss also the unusual temperature dependences.

12:15PM J23.00006 Magnetotransport properties and the Fermi surface of high-quality single crystal VB\(_3\), A.B. KARKI, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, D. GAUTREAUX, J.Y. CHAN, Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803, N. HARRISON, National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, NM 87545, D. BROWNE, R.G. GOODRICH, D.P. YOUNG, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803 — We have performed magnetotransport and dHvA measurements on high quality single crystals of VB\(_3\) grown from a molten aluminum flux. At low temperature the magnetoresistance (MR) of VB\(_3\) is very large (~1100%) and is found to be extremely sensitive to sample quality. The field dependence of the MR is proportional to the applied field squared, as is expected from open orbits on the Fermi surface. In addition, we have performed full potential LAPW calculations with the WIEN2K band package using the GGA density functional to compute the bands and Fermi surface. The calculations suggest that the area of the Fermi surface is a strong function of the lattice constants. The results of the calculations will be compared to experiment.

1:03PM J23.00010 Giant Fluctuations of the Coulomb Drag, BORIS NAROZHNY, The Abdus Salam ICTP, ADAM PRICE, ALEX SAVCHENKO, University of Exeter, DAVID RITCHIE, Cavendish Laboratory, University of Cambridge — Coulomb drag has been shown to provide information about electron-electron interactions not available from conventional conductance measurements, e.g. [1]. For mesoscopic conductors, a spectacular interference phenomenon is UCF. There has been a prediction that Coulomb drag should also show similar fluctuations: with decreasing temperature the fluctuations in the drag are expected to become larger than the average drag, resulting in a random change of the sign of the drag with varying carrier density [2]. Contrary to the UCF, the origin of these fluctuations involves both quantum interference and electron-electron interaction effects. Here we report the first observation of reproducible fluctuations of Coulomb drag in a double-layer GaAs structure, as a function of both the carrier density and magnetic field. Surprisingly, the observed fluctuations are almost four orders of magnitude larger than originally predicted in the theory, which considered diffusive transport of interacting electrons. We explain the observed enhancement by the fact that in ballistic transport, realised in our structures, the Coulomb drag probes the local properties of the system. The latter are expected to show much larger fluctuations than the global ones. [1] Gramila, Eisenstein, et al PRL 66, 1216 (1991). [2] Narozhny and Aleiner, PRL 84, 5383 (2000).
1:15PM J23.00011 Phase coherence of conduction electrons below the Kondo temperature\(^1\), GASEM M. ALZOUBI, NORMAN O. BIRGE, Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824-2320. — The scattering of conduction electrons by magnetic impurities is known as the Kondo effect. This effect has been the subject of theoretical and experimental investigations for several decades. Until very recently [1, 2], however, there was no theoretical expression for the temperature dependence of the inelastic scattering rate valid for temperatures \(T\) not too far below the Kondo temperature, \(T_K\). We present experimental measurements of the phase decoherence rate, \(\tau_\text{\tiny hop}^{-1}\), of conduction electrons in disordered dilute AgFe Kondo wires [3]. We compare the temperature dependence of the magnetic scattering rate, \(\gamma_m\), with a recent theory of dephasing by Kondo impurities [2]. A good agreement with theory is obtained for \(T/T_K > 0.1\). At lower \(T\), \(\gamma_m\), deviates from theory with a flatter \(T\)-dependence.


\(^1\)Supported by NSF DMR-0405238.

1:27PM J23.00012 Pre-Exponential factor and hopping criterion in the Efros-Shklovskii regime\(^1\), MIGUEL RODRIGUEZ, BONALDE ISMARDO, ERNESTO MEDINA, Centro de Física, IVIC — We address the variable-range hopping regime in the range for which the measured temperature \(T\) is of the order of the characteristic Efros-Shklovskii temperature \(T_{\text{ES}}\). In such a range current theories imply \(\tau_\text{\tiny hop}/\xi < 1\), where \(\tau_\text{\tiny hop}\) is the hopping length and \(\xi\) is the localization length, clearly in contradiction with the standard criterion for hopping conduction. We consider impurity-well wavefunctions of the form \(\psi(\mathbf{r}) \propto \exp(-r/\xi)\) and include the preexponential factor of the resistivity as a logarithmic correction in the Mott optimization procedure. From the general expression derived, the standard Efros-Shklovskii law is recovered for \(T \ll T_{\text{ES}}\); whereas an extended preexponential-dominated regime, consistent with \(\tau_\text{\tiny hop}/\xi > 1\), is found for \(T_{\text{ES}} \geq T\). We argue that the new expression resulting from an interplay between preexponential and exponential factors is a consistent extension of the classical Efros-Shklovskii argument.

\(^1\)Supported by FONACIT through grant G-97000670.

1:39PM J23.00013 Interaction Effects in a High-Mobility Two-Dimensional Electron Gas in a Nonquantizing Magnetic Field, TIGRAN SEDRAKYAN, EUGENE MISHCHENKO, MIKHAIL RAIKH, University of Utah — Two dimensional electron gas in a perpendicular nonquantizing magnetic field, \(B\), is considered. We demonstrate\(^2\) that the anomaly in the polarization operator, \(\Pi(q)\), near \(q = 2k_F\), where \(k_F\) is the Fermi momentum, gets smeared with \(B\) in a peculiar fashion: slowly decaying modulation, periodic in \((2k_F - q)^{3/2}\), emerges. The period of modulation sets a spatial scale, \(\rho_0^{-1} \propto B^{-2/3}\), which is much smaller than the Larmour radius, but much larger than the de Broglie wavelength. This scale manifests itself, e.g., in lifting the periodicity of the Friedel oscillations, \(\delta\rho(\mathbf{r})\) in magnetic field, namely we find that \(\delta\rho(\mathbf{r}) \propto \sin[(2k FR - (q\rho_0)^3)/12]/r^2\). The corrections to the interaction-induced characteristics of the 2D gas, such as relaxation rate and the tunnel density of states, coming from the distances \(\sim \rho_0^{-1}\), are shown to be strongly singular (as \(B^{1/3}\)) in magnetic field.

\(^2\)preprint cond-mat/0611111.

1:51PM J23.00014 Electric-Field-Induced Hopping Conductivity in Polymers, STEVEN HART, J.R. DENNISON, JERILYN BRUNSON, Utah State University — The resistivity of highly insulating polymers exhibits a dependence on electric field strength. Mott and Davis as well as Poole and Frankle describe theoretically the resistivity of disordered semiconductors, when subject to a changing electric field, in terms of hopping conductivity models. Although such models have often been applied to polymers, there is little direct experimental evidence to confirm the validity of these theories when applied to polymers. We present such results for a newly-developed block co-polymer Hytrel, a highly insulating material. The constant voltage resistivity test method has been used to study Hytrel for a range of electric fields approaching electrostatic breakdown. Previously taken preliminary measurements are suggestive that Hytrel validates hopping conductivity models. With additional data we consider whether the Hytrel results are consistent with existing models of electric-field induced hopping conductivity.

2:03PM J23.00015 Dephasing in a two-dimensional electron gas: System dependent, PHILIPPE JACQUOD, University of Arizona — We investigate dephasing in open ballistic chaotic systems in the limit of large system size to Fermi wavelength ratio, \(L/\lambda_F \gg 1\). Using the trajectory-based semiclassical theory, we calculate the weak localization correction \(g^{\text{WL}}\) to the conductance for a quantum dot coupled to (i) a dephasing voltage probe and (ii) an external closed quantum dot. In addition to the universal algebraic suppression \(g^{\text{WL}} \propto (1 + \tau_D/\tau_\phi)^{-1}\) with the dwell time \(\tau_D\) through the cavity and the dephasing rate \(\tau_\phi^{-1}\), we find an exponential suppression of weak localization by a factor \(\propto \exp[-\tilde{\tau}/\tau_\phi]\), with a system-dependent \(\tilde{\tau}\). In the dephasing probe model, \(\tilde{\tau}\) coincides with the Ehrenfest time, \(\tilde{\tau} \propto \ln[L/\lambda_F]\), in both cases of perfectly and partially transparent dot-lead couplings. In contrast, when dephasing occurs due to the coupling to an external dot, \(\tilde{\tau} \propto \ln[L/\xi]\) depends on the correlation length \(\xi\) of the coupling potential instead of \(\lambda_F\).

Tuesday, March 6, 2007 11:15AM - 2:15PM – Session J31 DCMP: Transport in Carbon Nanotubes: Experiment

11:15AM J31.00001 Transport in Carbon Nanotube – Polymer Field Emission Cathodes, DAVID CAREY, RICHARD SMITH, University of Surrey, NANOELECTRONICS GROUP TEAM — Embedding carbon nanotubes in host polymer matrices is an attractive way to control the nanotube density and provides a way to protect the nanotube emitter. Field emission from individual carbon nanotubes is usually discussed in terms of the field enhancement factor and electrostatic screening. The field enhancement factor can be regarded as the most important factor for efficient emission when transport of electrons is not the rate limiting step. Large area emission characterisation of cathodes tends to produce an ensemble average of the enhancement factor with sites with the lowest local turn on field emitting. We show that in nanotube polymer composites charge transfer through the composite and the effects of fluctuation induced tunneling due to variable nanotube-nanotube separation are important considerations.
A comparative study of transport properties between low- and high-resistance nanotube field-effect transistors — Swastik Kar, Aravind Vijayaraghavan, Caterina Soldano, Pulickel Ajayan, Rensselaer Polytechnic Institute — A large amount of fundamental work has been done in demonstrating the possibilities of using carbon nanotubes in future nanoscale devices. A primary concern in these devices has been the nature of transport mechanism in carbon nanotubes, especially semiconducting nanotubes where the conductance can be modulated significantly using a gate voltage, giving rise to a nanotube field-effect transistor. The quality of the metal-nanotube interface plays a significant role in determining the characteristics of field-effect transistors fabricated using single-wall carbon nanotubes. When contact-resistance is high due to a large Schottky barrier, the transistor characteristics are dominated by this barrier. When the barrier height is low, the intrinsic nanotube electronic properties determine the transistor characteristics. In this work, we compare and contrast the significant features of the transistor characteristics for the two types of devices.

Transport properties of metallic nanocluster impregnated multi wall carbon nanotubes — Caterina Soldano, Swastik Kar, Rensselaer Polytechnic Institute, SaiKAT Talapatra, Southern Illinois University, Saroj Nayak, Pulickel Ajayan, Rensselaer Polytechnic Institute — Artificially engineered low-dimensional heterostructures form a class of extremely exciting new materials for fundamental and applied research. One such very interesting system is the formation of arrays of metallic nanoclusters confined to one-dimension, within the scaffolding of another one dimensional material. A good example of this kind of a system is metal-nanocluster-impregnated carbon nanotubes. In this work, we report the fabrication of nanoscale heterostructures in the form of ferromagnetic metal nanocluster array impregnated multi wall carbon nanotubes. The nanoclusters can be impregnated into the nanotubes by a simple electrochemical technique. Two and four terminal devices with such individual nanoarchitectures have been fabricated using a combination of photo- and focused ion beam lithography. The systems form extremely exciting platforms for investigating charge and spin transport in confined geometries. We present preliminary data on the electrical properties of these novel systems at room and low temperatures.

Electronic transport in loops comprised of individual carbon nanotubes — JinsEong Heo, Gil Refael, Marc Bockrath, Caltech — We discuss electronic transport in loops comprised of individual carbon nanotubes. The conductance versus gate voltage shows oscillations with a number of periods. These oscillations persist up to temperatures ~50 K. We compare our results with a model [Dear APS organizers: please note the theoretical talk on the same subject given by Gil Refael. We would like to reference this talk if possible in this abstract.] that accounts for the interference of counterpropagating electron waves around the loop, analogous to a Sagnac interferometer in optics. In this model, the different velocities for right and left movers in the two carbon nanotube bands produce large energy scale interference oscillations. We find semi-quantitative agreement between our data and the theory. These results may enable phase coherence in nanotubes to be studied up to temperatures much higher than the cutoff imposed by thermal smearing.

Electronic transport across a Carbon nanotube Heterojunction: Experimental observations of high temperature Coulomb Charging and level spacing — Bhupesh Chandra, Yang Wu, Meninder Purewal, Mingyuan Huang, Hugen Yan, Linmin Huang, Stephen Brien, Tony Heinz, Philip Kim, James Hone, Columbia University — We present electrical transport measurements of individual a single-wall carbon nanotube in which the chiral indices (n, m) are not fixed along the nanotube length. These kinds of structures are known to show strong rectifying behavior in current voltage characteristics. At low temperatures the device essentially behaves like a quantum dot with very high charging energy and level-spacing. These features can be seen till 70K also, making it a high temperature single electron transistor.

Thermomagnetic Measurements of Transport in Single Walled Carbon Nanotubes — J. P. Heremans, The Ohio State University, Columbus OH 43210, C. M. Thrush, Delphi Research Laboratories, Shelby Township MI 48315, V. Jovovic, J. West, The Ohio State University, Columbus OH 43210 — The thermomagnetic transport properties of single walled carbon nanotubes bundles and mats in high magnetic fields have been measured in vacuum and in the presence of noble gases. They are used to determine mechanism responsible for change in thermopower and resistivity in the presence of gases with respect to one measured in high vacuum. The thermopower and its change in a magnetic field is recorded in Ne, Ar, Xe atmospheres. The variation of the zero-field thermopower with the presence of noble gases is consistent with that observed recently [1]. The magnetothermopower in a saturating magnetic field is only 0.2% larger than the zero-field thermopower. As the magnetothermopower in high field is independent of the scattering mechanism, this result argues in favor of diffusion mechanism as responsible for variations in transport properties, and against the recently suggested concept that collisions between gas molecules and the nanotubes are responsible for the changes in the thermopower. [1] H. E. Romero, K. Bolton, A. Tosen and P. C. Eklund, Atom Collision-induced Resistivity of Carbon Nanotubes, Science 307 89 (2005)

Observation of unusual structure in the low-temperature conductance of carbon nanotubes — Jeffrey D. Stephens, Jerome C. Licini, Lehigh University, A.T. Charlie Johnson, Douglas R. Strachan, Sam Khamis, Danvers E. Johnston, University of Pennsylvania — Carbon nanotubes grown by chemical vapor deposition on a oxidized silicon substrate were contacted to form a gated sample consisting of a pair of tubes in parallel. The sample was tested at low temperature and high magnetic field using a temperature single electron transistor.

Low temperature electron transport measurements of dielectrophoretically assembled single wall carbon nanotube — Paul Stokes, Liwei Liu, Saiful Khondaker, Nanoscience Technology Center and Department of Physics University of Central Florida — Dielectrophoretic (DEP) assembly of carbon nanotube (CNT) has attracted tremendous interests because of its usefulness in assembling CNT at selected positions in nanoelectronic circuits with high yield. Although DEP technique has been used to fabricate nanoelectronic devices, the effect of contact resistance and nanotube buckling at the electrode-substrate interface has not been examined. Here, we present electronic transport measurements of DEP assembled single wall carbon nanotubes from room temperature to 1.5 K to examine the contact resistance and nanotube buckling. The nanotubes were suspended in dimethylformamide (DMF) and assembled between gold or palladium electrodes by the application of an AC electric field. A fundamental understanding of the contact resistance and buckling behavior will lead to improved designing of DEP assembled devices.
1:03PM J31.00010 Electrical transport through tunable pn junctions in suspended carbon nanotubes , FERDINAND KUDEMTH, SHAHAL ILANI, P. L. MCEUEN, D. C. RALPH, Physics Dept., Cornell University, Ithaca, NY 14853 — Energy barriers play a crucial role within many carbon nanotube electronic devices, but their properties are often complicated by disorder induced by a substrate. Here we study well-controlled pn junctions in suspended carbon nanotubes whose transparency and position can be tuned using electrostatic gates. To achieve this we suspend individual single walled nanotubes above two separate gate electrodes and monitor the tube’s conductance while changing the gate voltages in various ways; by varying the voltage difference between both gates we can tune the pn junction’s width, whereas offsetting both gates by a common voltage controls its position. In small bandgap nanotubes we can additionally tune the junction’s transparency by axial magnetic fields. At low temperature, these devices allow measurements of quantum dots with a tunable length and coupling to the leads.

1:15PM J31.00011 Scaling of Resistance with Channel Length in Single Walled Carbon Nanotubes , MENINDER PUREWAL, Columbia University, Department of Applied Physics and Applied Mathematics, BYUNG HEE HONG, ANIRUDDH RAVI, Columbia University, Department of Physics, BHUPESH CHANDRA, JAMES HONE, Columbia University, Department of Mechanical Engineering, PHILIP KIM, Columbia University — We report on the scaling of resistance with channel length in single walled carbon nanotubes (SWNTs) with multiple PdOhmic contacts. The channel lengths range from 100nm to 400um. The intrinsic 1-D resistivity of individual SWNTs are measured from the slope of the linear dependence of resistance and length. The temperature dependent electron mean free length can be obtained from these data. While the mean free length ranges 100-500 nm at room temperature, the low temperature saturated value shows values as high as ∼10um. In addition, we will discuss possible mechanisms for the deviation from linear scaling behavior, as seen in long length scales (>100um). Finally, we will report unusual strong suppression of conductance outside of the band gap regions of several SWNTs deviating from typical small and large band gap semiconducting SWNTs.

1:27PM J31.00012 Magnetic and Transport Properties of Carbon Nanotube-Based One-Dimensional Nanocomposite Materials , ADAM FRIEDMAN, LATIKA MENON, JESSE SILVERBERG, Northeastern University Department of Physics, YUNG JOON JUNG, Northeastern University Department of Mechanical Engineering — Carbon nanotubes (CNTs) prove to be extremely well suited for the investigation of electron conduction in one-dimensional materials. CNTs have been shown to conduct in the ballistic regime according to Landauer’s formula. When placed in electromagnetic fields and at low temperatures where the mean free path is smaller than the diameter of the tube, CNTs been shown to be the perfect platform to study Luttinger liquid behavior, the Kondo effect and quantum fluctuations, electron coherence, and the Aharonov-Bohm effect. These unique properties can be further enhanced by inserting materials into the cavities of the CNTs. In this work, we use anodized porous alumina templates as a substrate for the controlled growth of CNTs by means of chemical vapor deposition. AC electrodeposition is then used to deposit Fe, Ni, Co, as well as semiconductor nanowires inside the tubes. The magnetic and electrical properties of such nanotube-nanowire composites (both single and bundled) in the presence of applied magnetic fields up to 5.5T and at low temperatures down to 4.2K are studied and preliminary results will be reported.

1:39PM J31.00013 One-Dimensional Carbon Nanotube Electrodes , CARLA AGUIRRE, BENIOFT ST. ANTOINE, Departement de Genie Physique, Ecole Polytechnique de Montreal, MATHIEU PAILLET, Departement de Chimie, Universite de Montreal, PATRICK DESJARDINS, Departement de Genie Physique, Ecole Polytechnique de Montreal, RICHARD MARTEL, Departement de Chimie, Universite de Montreal — The study of the transport properties of organic semiconducting materials has been limited by the lack of suitable electrical contacts. Inappropriate charge injection at the electrode - organic semiconductor interface results in large contact resistances that often dominate device performance. We describe a strategy for circumventing charge injection barriers by using 1D metallic carbon nanotube electrodes. The favorable electrostatics at the tip of an individual carbon nanotube allows for efficient field assisted charge injection into organic semiconducting layers. A detailed finite element numerical study has allowed us to determine the scaling parameters required to optimize the performance of carbon nanotube electrodes. We present experimental results for pentacene thin-film transistors connected using individual metallic carbon nanotube source and drain contacts. Different gate oxide thicknesses (20 - 100 nm), channel lengths ( 2 - 100 nm) and carbon nanotube diameters (1 - 3 nm) were explored using experimental and numerical techniques.

1:51PM J31.00014 Heat Transport in Carbon Nanotubes Measured using Raman Spectroscopy , I-KAI HSU, University of Southern California, MICHAEL PETTES, The University of Texas at Austin, RAJAY KUMAR, University of Southern California, LI SHI, The University of Texas at Austin, STEPHEN CRONIN, University of Southern California — We investigate thermal transport in suspended carbon nanotubes on micromachined heating devices using Raman spectroscopy. Individual carbon nanotubes suspended between two membranes with integrated heaters and thermometers are characterized using micro-Raman spectroscopy. The temperature dependent shifts of the Raman mode frequencies are used to quantify the heating along the length of the nanotube. We find that results vary depending on the number of defects in the nanotube. The results are understood on the basis of a diffusive thermal transport model.

2:03PM J31.00015 Breakdown of Fourier’s law in nanotube thermal conductors , CHIH-WEI CHANG, DAVID OKAWA, HENRY GARCIA, ARUNAVA MAJUMDAR, ALEX ZETTL, Physics Department, University of California at Berkeley — We present experimental evidence that the room temperature thermal conductivity (κ) of individual multiwall carbon nanotubes and boron-nitride nanotubes does not obey Fourier’s law as do ordinary thermal conductors. By varying the length (L) of the nanotube, we find that κ diverges as L^{1.0-1.9}. Our results show that Fourier’s law is violated despite the fact that the ballistic phonon condition is not satisfied and large isotopic disorder is present.

Tuesday, March 6, 2007 2:30PM - 5:30PM — Session L1 DCMP DMP: Basic Research Needs for Superconductivity Colorado Convention Center Four Seasons 2-3

2:30PM L1.00001 Superconductivity: Challenges and Opportunities 1 , J.L. SARRAEO, Los Alamos National Laboratory — As part of its effort to define transformational opportunities for fundamental research in energy security, the Department of Energy’s Office of Basic Energy Sciences held a workshop on Basic Research Needs for Superconductivity. The workshop identified a number of materials grand challenges and priority research directions for transforming the power grid to meet the needs of the 21st century. The prospect of moving from materials by serendipity to materials by design and of advancing the frontiers of epistemic science to yield higher performing nano-structured architectures are two of the these challenges that could impact superconductivity research specifically and materials research more broadly. In this talk we highlight recent technical successes that motivate and illustrate these opportunities. We also discuss the science that might be necessary to accomplish these goals in the hopes of nucleating further community input and engagement. In collaboration with Wai Kwok, Argonne National Laboratory.

3:06PM L1.00002 Approaches to New Superconducting Materials

JAMES ECKSTEIN, Department of Physics and Fredrick Seitz Materials Research Laboratory, University of Illinois, Urbana — Over the last twenty years a large set of new superconductors with extraordinary properties have been discovered and studied. They are all by any measure complex materials, involving several elements arranged in complex crystal structures. Even the normal states of these materials exhibit highly correlated behavior, and the superconducting states are equally unusual, with complex order parameter symmetries, exotic vortex behavior and strong dependence on carrier doping. In the future, new complex materials that are chemically stable compounds will certainly continue to be found, at least some of which may result from rational searches. There is also an opportunity to create new materials in which the molecular, electronic, spin and phonon structure that sets the stage for the emergence of a superconducting state is defined artificially. Such "meta-materials" allow for the factors that are important for an emergent state to be included in new ways, and they also provide a test bed for predictive theory. Oxides are particularly well suited for this kind of work, since heterostructures between different phases can be formed in many cases with little disorder. In other correlated systems, some new and useful properties not found in naturally occurring compounds have been engineered this way by researchers in several labs. Many heterostructure issues governing the resulting electronic and magnetic structure remain to be systematically studied, including state line-up, charge transfer, interface composition and bond energies to name a few.

3:42PM L1.00003 Structure and Dynamics of Vortex Matter

WAI-KWONG KWOK, Argonne National Laboratory — The DOE Basic Energy Sciences Workshop on Basic Research Needs for Superconductivity identified grand challenges and research priorities for discovery and use inspired basic research to transform the US power grid to meet the needs of the 21st century. Vortex matter research is central to this endeavor and helps support both fundamental and applied research. The science of vortex matter embodies the fundamental mysteries of vortex-vortex interactions in an inhomogeneous and anisotropic matrix. Understanding the complex phase diagrams and the dynamic responses that result from these competing effects is an outstanding challenge. Simultaneously, the prospect of controlling these interactions opens new horizons for basic research such as the development of a microscopic theory for vortex dynamics, exploration of vortex nucleation at magnetic and superconducting interfaces and designs for pinning a vortex liquid at high temperatures. This presentation will highlight ways in which nanotechnology based methodologies, dynamic vortex creep phenomena and powerful computer simulations play a role in enhancing our understanding of next-generation and new classes of superconductors.

4:18PM L1.00004 Understanding of Mechanisms for Design of Advanced Superconductors

WARREN PICKETT, University of California Davis — A recent DOE panel considered the future of research in superconducting materials and made a number of recommendations for priority research directions (http://www.ex.doe.gov/kes/reports/files/SC_rpt.pdf), two of which will be discussed. These items, under the rubric of Enabling Superconductivity, emphasize that Finding the Mechanisms is essential for furthering the field, and that once understood, the prospect of Superconductors by Design becomes a viable line of research. Establishing the mechanism in the high temperature superconducting cuprates continues to attract substantial efforts, with no consensus near. In several superconductors, including some discovered in the past decade or so, having Tc around or above 20 K ([BaNiO2]2, Li_HNCI, PuCoGa5) the mechanism is in question. On the more positive side, there are several cases established in the past six years, beginning with MgB2 and extending to elemental metals under pressure (Li, Y, Ca), where the familiar electron-phonon mechanism has provided unexpectedly high Tc and thereby stimulated enthusiasm and optimism into this area of superconductivity research. The clear understanding of this mechanism (at least in many respects) provides a path for improvements in superconducting materials.

4:54PM L1.00005 Transforming the Grid with Superconductivity

ALEXIS MALOZEMOFF, American Superconductor Corporation — The electric power grid in the United States faces critical challenges: overloading caused by years of limited investment and steady load growth, bottlenecks in power corridors into urban centers, voltage instability leading to brownouts and blackouts, growing fault currents in large urban and suburban areas, as well as the need for increased efficiency. Power equipment based on high temperature superconductors (HTS) offers solutions to these challenges: high capacity, non-interfering HTS cables addressing power bottlenecks, HTS fault current limiters controlling fault currents, HTS synchronous condensers and novel controllability features of HTS cables which address stability issues, HTS transformers and generators with increased efficiency. A variety of commercial-level demonstrations make the impact of HTS power equipment imminent.

Tuesday, March 6, 2007 2:30PM - 5:30PM –
Session L3 DCMP: Novel Phenomena in Granular Systems with Complex Interactions Colorado Convention Center Korbel 2A-3A

2:30PM L3.00001 Thresholds and Dynamics for Oscillating Granular Layers

JERRY GOLLUB, Haverford/Penn — The onset and dynamics of flow in shallow horizontally oscillating granular layers are studied and compared to the behavior of avalanches. The variation with depth of the starting acceleration for the oscillating layer matches (approximately) the corresponding variation of the tangent of the starting angle for avalanches in the same container at low frequencies, but deviates as the frequency is increased. However, the threshold behavior depends significantly on the measurement protocol. Just above threshold, the motion decays with time as the material re-organizes over a minute or so, causing the apparent threshold to increase. Once excited, the rheology of the material is found to vary in time during the cycle in surprising ways. If the maximum inertial force (proportional to the container acceleration amplitude) is slightly higher than that required to produce flow, the flow velocity grows as soon as the inertial force exceeds zero in each cycle, but jamming occurs long before the inertial force returns to zero. At higher acceleration, the motion is fluidic-like over the entire cycle. However, the fraction of the cycle during which the layer is mobile is typically far higher than what one would predict from static considerations or the behavior of the inclined layer. Finally, we consider the flow profiles as a function of both the transverse distance across the cell at the free surface, and also as a function of the vertical coordinate in the boundary layer near the sidewall. These profiles have time-dependent shapes, and are therefore significantly different from profiles previously measured for avalanche flows.

Supported by NSF-DMR.
In this work we focus on the mechanical interaction among non-motile bacteria in engineered biofilms. These biofilms are formed by growing two-dimensional bacterial colonies in a highly controlled microfluidic environment. We combine experimental observations and analysis with discrete-element molecular dynamics simulations and theoretical modeling to provide mesoscopic description of the biofilm growth. Our results reveal how cell growth and colony expansion trigger the formation of the orientational (nematic) order in the biofilms.


3:06PM L3.00002 Particle Shape and Dynamics of Granular Matter: Swarming to Swirling

ARSHAD KUDROLLI, Department of Physics, Clark University, Worcester, MA 01610 — We will discuss a series of experiments performed with granular rods, dimers, and flexible chains on a vibrated plate to illustrate the effect of particle shape on self-organization. A non-spherical shape is shown to lead to not only states which resemble nematic and smectic phases but also causes novel dynamics [1]. The ratchet mechanism which leads to vortex motion in a collection of rods on a vibrated plate and drift motion in a bouncing dimer will be discussed [2, 3]. The friction at the point of contact between particle and the substrate, and the coupling about the center of mass of a non-spherical is proposed to lead to observed motion. Exploiting this mechanism we construct mechanical self-propelled particles (SPP) using rods with asymmetric mass distributions. We then investigate the SPP number fluctuations, flow fields, and orientation order inside a container as a function of number density and excitation, and compare their statistics with recent models of active nematic particles and living cells.


3:42PM L3.00003 Externally driven magnetic granular layers at a liquid/air interface: self-organization, flows and magnetic order

ALEXKEY SNEZHKO, Argonne National Laboratory — Collective dynamics and pattern formation in ensembles of magnetic microparticles suspended at the liquid/air interface and subjected to an alternating magnetic field are studied. Experiments reveal a new type of nontrivially ordered dynamic self-assembled structures ("snakes") emerging in such systems in a certain range of field magnitudes and frequencies. These remarkable structures are directly related to surface waves in the liquid generated by the collective response of magnetic microparticles to the alternating magnetic field. In addition, a large-scale vortex flows are induced in the vicinity of the dynamic structures. Some features of the self-localized snake structures can be understood in the framework of an amplitude equation for parametric waves coupled to the conservation law equation describing the evolution of the magnetic particle density. Self-assembled snakes have a complex magnetic order: the segments of the snake exhibit long-range antiferromagnetic ordering mediated by the surface wave, while each segment is composed of ferromagnetically aligned chains of microparticles. A phenomenological model describing magnetic behavior of the magnetic snakes in external magnetic fields is proposed.

4:18PM L3.00004 Nonlinear dynamics of semiflexible magnetic filaments in an external ac magnetic field

ANDREJS CEBERS, University of Latvia — Chains of magnetic particles exist in nature (magnetotactic bacteria, magnetic colloids) and can be created artificially by linking magnetic particles with some polymer (PAA,DNA). Theoretical description of magnetic filaments is based on models of semiflexible polymers extended by incorporation of the effects of body torques due to long-range magnetic interactions. On the basis of these models different phenomena are described - buckling due to body torques, self-propulsion in an AC field, tumbling in the shear flow, orientation of ferromagnetic filaments in the direction perpendicular to an AC field, liquid flow excited by oscillating in an AC field tips of magnetic filaments floating on the surface of the liquid and others. Connection of equilibrium shapes of magnetic filaments with solutions of elastic and plastic behavior is established. Different regimes of magnetic response of the suspension of magnetic filaments are analyzed by taking into account the thermal noise.

1 Supported by UL grant 2006/1-229701.
2 In collaboration with M. Belovs, K. Erglis, and A. Sharipo.

4:54PM L3.00005 Nematic Ordering in a Population of Growing and Dividing Rod-like Cells

LEV TSIMRING, University of California, San Diego — Morphogenesis is one of the most important themes in biology, and it is also central to nonequilibrium physics. The fundamental issue is to understand how local interactions of elementary components lead to collective behavior and the formation of a highly organized system. In nature this self-organization is found on many different scales, from single cells to schools of fish and herds of animals. Collective behavior leads to significant selective advantages for living organisms. At low density, communication among cells occurs mainly due to chemotaxis, the mechanical response of cell to the gradients of chemicals emitted by other cells. At higher densities, steric exclusion effects may strongly affect their collective behavior. In this work we focus on the mechanical interaction among non-motile bacteria in engineered biofilms. These biofilms are formed by growing two-dimensional bacterial colonies in a highly controlled microfluidic environment. We combine experimental observations and analysis with discrete-element molecular dynamics simulations and theoretical modeling to provide mesoscopic description of the biofilm growth. Our results reveal how cell growth and colony expansion trigger the formation of the orientational (nematic) order in the biofilms.

1 In collaboration with D. Volfs, S. Cookson, and J. Hasty, University of California, San Diego.

Tuesday, March 6, 2007 2:30PM - 5:30PM –
Session L4 DCMP GQI: DCMP / GQI Prize Session Colorado Convention Center Korbel 2B-3B

2:30PM L4.00001 Quantum Measurement with the Josephson Bifurcation Amplifier

IRFAN SIDDIQI, UC Berkeley — The Josephson tunnel junction is a unique dipolar circuit element which can be both non-linear and non-dissipative. This combination makes it well suited to measuring quantum systems since non-linearity enables fast, sensitive detection while the absence of dissipation reduces loss of coherence. When the junction is driven close to a bifurcation point with a sufficiently intense microwave drive, then two metastable states exist which differ in oscillation amplitude and phase. The junction remains confined to a single well of its sinusoidal potential in both of these states and no DC voltage is generated. The oscillation state of the junction can be determined by measuring either the reflected or transmitted AC microwave drive signal. The transition between these dynamical states is a sensitive function of the junction critical current. Therefore, the critical current serves as the input variable of the amplifier and can be modulated by the application of a magnetic flux, electric charge, or a superconducting phase. The bifurcation amplifier has been successfully used for the state readout of superconducting qubits, and has many potential applications including the coherent detection of magnetic nanostructures such as single molecule magnets.

3:06PM L4.00002 Prize for Research at an Undergraduate Institution Talk: A Discrete Wigner Function

WILLIAM WOOTTERS, Williams College — For a quantum particle moving in one dimension, the Wigner function represents the particle’s quantum state as a real function on the two-dimensional phase space. Though the Wigner function typically takes negative values and can therefore not be interpreted as a probability distribution, its integral along any axis in phase space—even a skew axis—is in fact the probability distribution of an observable associated with that axis. A number of authors have developed generalizations of the Wigner function that apply to discrete quantum systems, but such generalizations are often problematic when the state-space dimension is even. Here we present a discrete Wigner function that shares with the continuous Wigner function the “tomographic” property described above, and is well suited to describe a system of binary quantum objects. We discuss potential applications to quantum computation and quantum cryptography.
Results suggest the potential for practical utilization of electrically generated spin polarization in room temperature semiconductor devices.

Spin-dependent scattering mechanism. Both the current-induced spin polarization and the spin Hall effect are robust to room temperature in ZnSe. These indicative of the spin Hall effect. The spin Hall conductivity is estimated according to a spin accumulation model and is found to be consistent with the extrinsic exhibit both in-plane bulk current-induced spin polarization and an out-of-plane spin accumulation of opposite sign on opposite edges of a conducting channel field is studied and found to only be measurable in strained layers, likely due to the weak spin-orbit interaction in ZnSe. Despite this, unstrained n-ZnSe layers reduction of the spin accumulation at the edges of a spin Hall bar, even when the spin current is zero. We have also pointed out that the relative size of the SJ contribution remains completely unaffected by Coulomb scattering. The different behaviors of the SS and SJ contributions result in a Coulomb-induced SS contribution is significantly reduced by the spin Coulomb drag – the Coulomb friction between electrons of opposite spin orientations. At the same time, the SJ contribution contributes result in a Coulomb-induced reduction of the spin accumulation at the edges of a spin Hall bar, even when the spin current is zero. We have also pointed out that the relative size of the SJ and SS contributions depends on mobility and we have proposed an experiment to distinguish between the two [2].

The spin-Hall effect is the generation of a steady spin current perpendicular to an externally imposed d.c. electric field. The effect is driven by spin-orbit interactions but its details are influenced by several processes like electron-impurity scattering, electron-electron scattering, and spin precession. In this talk I describe our recent work on the role of electron- electron scattering in the spin Hall effect in an n-type [110] GaAs quantum well, where spin precession is absent. We have studied the spin Hall conductivity (SHC) by a combination of the Boltzmann equation and the Kubo formula for the spin current [1], [2]. The two main contributions to the SHC – “skew scattering” (SS) and “side-jump” (SJ) – respond very differently to the inclusion of Coulomb interactions. The SS contribution is significantly reduced by the spin Coulomb drag – the Coulomb friction between electrons of opposite spin orientations. At the same time, the SJ contribution remains completely unaffected by Coulomb scattering. The different behaviors of the SS and SJ contributions result in a Coulomb-induced reduction of the spin accumulation at the edges of a spin Hall bar, even when the spin current is zero. We have also pointed out that the relative size of the SJ and SS contributions depends on mobility and we have proposed an experiment to distinguish between the two [2].

Work supported by NSF Grant No. DMR-0313681.

3:42PM L4.00003 Atoms in a Cavity: A Source of Narrowband Photon Pairs, HUANQIAN LOH, Data Storage Institute — Coupling atoms to an optical cavity can significantly enhance the directionality of photon emission from atoms. Using such an atoms-cavity system, we have created a high-brightness source of narrowband, identical-photon pairs. The source was applied to two experiments: interferometry and entanglement. Biphoton interferometry holds promise to demonstrate precision beyond the shot noise limit, although the measured interference fringe visibility of 0.84 ± 0.04 only translated to a shot noise limited phase uncertainty. Polarization-time entangled photon pairs were also directly generated via an adjusted optical pumping scheme for the atoms.

4:18PM L4.00004 Low-temperature infrared spectroscopy of H₂ in solid C₆₀(1), HUGH CHURCHILL, Harvard University — Diffuse reflectance infrared spectroscopy was used to probe the quantum dynamics of H₂ trapped in a C₆₀ lattice. Because free H₂ is infrared inactive, features of the infrared spectra are induced solely through interactions with the host material and as such provide detailed information about the potential at the binding site. The design and construction of a cryogenic apparatus allowed the extension of previous room temperature measurements to temperatures as low as 10 K at pressures as high as 100 atm. The low temperature spectra contained much sharper peaks and a rich fine structure, enabling more precise determination of the details of the C₆₀-H₂ interaction potential. These studies of H₂ in C₆₀ inform hydrogen storage materials research in a broader context, as illustrated by the diffuse reflectance spectra of H₂ in MOF-5.

4:54PM L4.00005 Maximum entropy-principle approach to quantum storage in strongly correlated systems, FAZLEY BARY MALIK, Southern Illinois University Carbondale — We shall investigate whether it is possible to generate QUBITS and/or QUTRITS starting with a modified version of Hubbard-Anderson Hamiltonian pertinent to describe magnetic properties of strongly correlated systems, particularly manganites. For this purpose, we shall derive the expressions for expectation values of a set of relevant operators starting with the Shannon entropy and using maximum entropy principle. It also allows us to derive Weiss relation that relates the spin-projection at a site to the interaction of that site with the rest of the medium. In the presence of an internal or applied magnetic field, or both, the absolute minima of free energy for spin projection in z-direction is +1, 0 and -1 for a triplet pair of fermion at three different temperatures, which are identified as QUBITS (in case one does not distinguish between ±1 projections) or QUTRITS.

Tuesday, March 6, 2007 2:30PM - 5:30PM —
Session L5 DCMPC: Spin Manipulation in Semiconductors and Metals for Spintronics, Colorado Convention Center Korbel 1A-1B

2:30PM L5.00001 Coulomb Interaction in the Spin-Hall Effect, EWELINA HANKIEWICZ, University of Missouri-Columbia — The spin-Hall effect is the generation of a steady spin current perpendicular to an externally imposed d.c. electric field. The effect is driven by spin-orbit interactions but its details are influenced by several processes like electron-impurity scattering, electron-electron scattering, and spin precession. In this talk I describe our recent work on the role of electron-electron scattering in the spin Hall effect in an n-type [110] GaAs quantum well, where spin precession is absent. We have studied the spin Hall conductivity (SHC) by a combination of the Boltzmann equation and the Kubo formula for the spin current [1], [2]. The two main contributions to the SHC – “skew scattering” (SS) and “side-jump” (SJ) – respond very differently to the inclusion of Coulomb interactions. The SS contribution is significantly reduced by the spin Coulomb drag – the Coulomb friction between electrons of opposite spin orientations. At the same time, the SJ contribution remains completely unaffected by Coulomb scattering. The different behaviors of the SS and SJ contributions result in a Coulomb-induced reduction of the spin accumulation at the edges of a spin Hall bar, even when the spin current is zero. We have also pointed out that the relative size of the SJ and SS contributions depends on mobility and we have proposed an experiment to distinguish between the two [2]. [1] E. M. Hankiewicz and G. Vignale Phys. Rev. B 73, 115339 (2006) [2] E. M. Hankiewicz, G. Vignale and M. E. Flatté cond-mat/0603144 (PRL in press)

3:06PM L5.00002 Electrically-Induced Polarization and the Spin Hall Effect in Semiconductors at Room Temperature, NATHANIEL STERN, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — The capability to generate and manipulate spin polarization through the spin-orbit interaction inspires growing interest in all-electrical techniques to exploit electron spins for applications in semiconductor spintronics. Experiments show spin polarization can be electrically generated by current-induced spin polarization from internal magnetic fields in the bulk of a conducting channel, or accumulation of spin polarization near sample edges due to transverse spin currents generated by the spin Hall. These spin currents can drive spin accumulation over micron length scales in semiconductor arms transverse to a conducting channel.

More recently, we investigate electrically generation of spin polarization in n-ZnSe epilayers using Kerr rotation spectroscopy. The internal magnetic field is studied and found to only be measurable in strained layers, likely due to the weak spin-orbit interaction in ZnSe. Despite this, unstrained n-ZnSe layers exhibit both in-plane bulk current-induced spin polarization and an out-of-plane spin accumulation of opposite sign on opposite edges of a conducting channel indicative of the spin Hall effect. The spin Hall conductivity is estimated according to a spin accumulation model and is found to be consistent with the extrinsic spin-dependent scattering mechanism. Both the current-induced spin polarization and the spin Hall effect are robust to room temperature in ZnSe. These results suggest the potential for practical utilization of electrically generated spin polarization in room temperature semiconductor devices.

Work supported by the NSF, ONR, and the Hertz Foundation.


3:42PM L5.00003 Spin Transport and Scattering in Ferromagnetic Semiconductor Heterostructures1
NITIN SAMARTH, Dept. of Physics, The Pennsylvania State University — A fundamental understanding of the transport and scattering of spin-polarized carriers in semiconductors is central to the development of semiconductor spintronics. We describe recent work that probes the spin-dependent transport of holes in heterostructures derived from the ferromagnetic semiconductor (Ga,Mn)As. In tensile-strained (Ga,Mn)As/(In,Ga)As heterostructures with perpendicular magnetic anisotropy, we observe a longitudinal magnetoresistance that is antisymmetric in magnetic field and attributed to slowly propagating magnetic domain walls [1]. This is confirmed both by a simple calculation and by measuring patterned submicron channels designed to trap single domain walls. In (Ga,Mn)As/p-GaAs/(Ga,Mn)As trilayer heterostructures, we demonstrate an all-semiconductor spin-valve effect, despite short spin-diffusion and elastic scattering lengths in the spacer layer [2]. Magnetoresistance (MR) measurements carried out in the current-in-plane geometry reveal positive MR peaks when the two ferromagnetic layers are magnetized orthogonal to each other. Measurements with different post-growth annealing conditions and spacer layer thickness show that the positive MR originates in a noncollinear spin valve effect due to spin-dependent scattering at interfaces.


1Supported by NSF and ONR

4:18PM L5.00004 Electrical detection of spin transport in lateral ferromagnet-semiconductor devices1
XIAOHUA LOU, University of Minnesota — A fully electrical scheme of spin injection, transport, and detection in a single ferromagnet-semiconductor structure has been a long-standing goal in the field of spintronics. In this talk, we report on an experimental demonstration of such a scheme. The devices are fabricated from epitaxial Fe/GaAs (100) heterostructures with highly doped GaAs as a Schottky tunnel barrier. A set of closely spaced Fe contacts on the top of an n-GaAs channel are used as spin injectors and detectors. Reference electrodes are placed at the far ends of the channel, allowing for non-local spin detection [1]. The electro-chemical potential of the detector is sensitive to the relative magnetizations of the injector and detector. In spin-valve measurements, a magnetic field is applied along the Fe easy axis to switch the relative magnetizations of injector and detector from parallel to antiparallel, resulting in a voltage jump that is proportional to the non-equilibrium spin polarization in the channel. A more rigorous test of electrical spin detection is the agreement with the spin-dependent non-local voltage. Both the transport and optical measurements show a non-linear relationship between the bias voltage at (reverse bias at the injector) or spin accumulation (forward bias at the injector) is measured using the magneto-optical Kerr effect and is found to be in good agreement with the spin accumulation (forward bias at the injector) is measured using the magneto-optical Kerr effect and is found to be in good agreement with the spin-dependent non-local voltage. Both the transport and optical measurements show a non-linear relationship between the bias voltage at the injector and the spin polarization in the channel. [1] M. Johnson and R. H. Silsbee, Phys. Rev. Lett. 55, 1790 (1985).

1This work was done in collaboration with C. Adelmann, S. A. Crooker, E. S. Garlid, J. Zhang, S. M. Reddy, S. D. Flexner, C. J. Palmstrøm, and P. A. Crowell and was supported by the NSF MRSEC program and ONR.

4:54PM L5.00005 Current-induced domain wall motion in ferromagnetic semiconductors1
HIDEO OHNO, Tohoku Univ./ ERATO, JST — Low magnetization (~0.05 T) and high spin-polarization in ferromagnetism of transition metal-doped GaAs allow us to explore a number of spin-dependent phenomena not readily accessible in metal ferromagnets. Spin-polarized current induced domain wall (DW) motion in (Ga,Mn)As [1, 2] reveals rich physics resulting from the interaction between spin-polarized electrons and localized spins inside a magnetic DW. By using a 30 nm thick (Ga,Mn)As layer ($x_{CFA} = 0.045$) with perpendicular magnetic anisotropy, we have measured by magneto-optical Kerr microscopy a wide range of velocity-current density curves in the sample temperature range of 97 – 107 K. Two regimes are found in the current density dependence of the DW velocity. At high-current densities (> $2 \times 10^9$ A/cm$^2$), the domain wall velocity is approximately a linear function of the current density above a threshold current density. This result will be compared to the recent theories of DW motion. At low-current densities, the functions $v(w)$ of the velocity-current curves follow an empirical scaling law, obtained by modifying the one for magnetic-field induced creep. This shows that current-induced DW creep is present. We have also determined the intrinsic resistance of the DW in a similar configuration [3].

1 Supported work with M. Yamanouchi, D. Chiba, F. Matsukura, and T. Dietl. Partly supported by the IT-Program of RR2002 by MEXT.

4. Work done with M. Yamanouchi, D. Chiba, F. Matsukura, and T. Dietl. Partly supported by the IT-Program of RR2002 by MEXT.

Tuesday, March 6, 2007 2:30PM - 5:30PM –
Session L8 DCMP: Superconductivity Theory: Strongly Correlated Systems Colorado Convention Center Korbel 1C

2:42PM L8.00002 Superfluid Stiffness, Nodal Quasiparticles and Quantum Phase Fluctuations in Underdoped Cuprates, NANDINI TRIVEDI, RAJDEEP SENSARMA, MOHIT RANDERIA, The Ohio State University — We study the low temperature superfluid stiffness $\rho_s(T, x)$ as a function of hole doping $x$ and temperature $T$ for strongly correlated $d$-wave superconductors. Using Gutzwiller projected wavefunctions and renormalized mean-field theory (RMFT), we calculate $\rho_s(0; x)$ and show that it scales with the quasiparticle spectral weight $Z$. These analytical results are in excellent agreement with earlier variational Monte Carlo studies [1]. We next show that self-consistent inclusion of the zero point motion of phase fluctuations leads to further suppression of $\rho_s(0; x)$, which now vanishes below a doping level of approximately 5%. To determine the $T$-dependence of $\rho_s$, we calculate the current carried by nodal quasiparticles (QP) within RMFT and show that the effective charge of the nodal QP is given by $2m^*/m$. Our analytic formula for the effective charge is in excellent agreement with numerical Monte Carlo results of Nave et al. [2]. We will conclude by comparing our results with experiments on underdoped cuprates.


2:54PM L8.00003 Phenomenological theory of the underdoped phase of a high-$T_c$ superconductor, ALEXEI TSVELIK, Brookhaven National Laboratory, ANDREY CHUBUKOV, University of Wisconsin, Madison — We model the Fermi surface of the cuprates by one-dimensional nested parts near $(0, \pi)$ and $(0, 0)$ and unnested parts near the zone diagonals. Fermions in the nested regions form 1D spin liquids, and develop spectral gaps below some $\sim (0)

2:06PM L8.00004 Competing ferromagnetism in high temperature copper oxide superconductors, SUDIP CHAKRAVARTY, ANGELA KOPP, AMIT GHOSAL, UCLA — While much attention has been paid to the underdoped regime of the hole-doped cuprates because of its proximity to a complex Mott insulating phase, little attention has been paid to the overdoped regime. Experiments are beginning to reveal that the phenomenology of the overdoped regime is just as puzzling. For example, the electrons appear to form a Fermi liquid, but this interpretation is problematic: any trace of Mott phenomena, as signified by incommensurate antiferromagnetic fluctuations, is absent, and the uniform spin susceptibility shows a ferromagnetic upturn. Here we show and justify that many of these puzzles can be resolved if we assume that competing ferromagnetic fluctuations are simultaneously present with superconductivity, and the termination of the superconducting dome in the overdoped regime marks a quantum critical point beyond which there should be a genuine ferromagnetic phase at zero temperature. We propose new experiments, and make new predictions, to test our theory and suggest that effort must be mounted to elucidate the nature of the overdoped regime, if the problem of high temperature superconductivity is to be solved.

3:06PM L8.00005 Theory of Infrared Hall Conductivity of Electron-doped Cuprates, JIE LIN, ANDREW MILLIS, Department of Physics, Columbia University — It has been proposed by several experiments that the electron-doped cuprate Pr$_{2-x}$Ce$_x$CuO$_{4+y}$ undergoes a quantum phase transition to an antiferromagnetic state for the doping $x$ smaller than 0.16. Here, we investigate the infrared Hall conductance of the electron-doped cuprates in the commensurate spin density wave state, using the linear response theory. The qualitative agreement between our results and the available experimental data provides strong evidence in favor of the spin density wave scenario and suggests that the magnitude of the gap is large, while quantitative discrepancies point towards additional physics which may be related to scattering of carriers off spin fluctuations. We also discuss the Hall conductivity sum rule and its connection to the experiments.

3:18PM L8.00006 Strong correlations lead to protected low energy excitations in disordered $d$-wave superconductors, ARTI GARG, Technion, Israel Institute of Technology, MOHIT RANDERIA, NANDINI TRIVEDI, The Ohio State University — We show that strong correlations play a vital role in protecting low energy excitations in disordered high temperature superconductors. The impurity-induced low-energy density of states (DOS) is greatly reduced in the strongly correlated superconductor compared to $d$-wave Bogoliubov-deGennes theory which ignores strong correlations. The gapless nodal quasiparticles, and the resulting $\nu$ in the low-energy DOS, are much more robust against disorder compared to the large-gap antinodal excitations. We discuss the relevance of our results to angle-resolved photoemission and scanning tunneling spectroscopy experiments. Reference: A. Garg, M. Randeria, and N. Trivedi, cond-mat/0609666

3:24PM L8.00007 Electron-phonon renormalization in Cuprates, PEIHONG ZHANG, University at Buffalo, SUNY, STEVEN G. LOUIE, MARVIN L. COHEN, UC Berkeley — Electron-phonon (e-ph) renormalization effects in a model cuprate system, CaCuO$_2$, are studied by employing density functional theory based methods. Whereas calculations based on the local spin density approximation (LSDA) predicts negligible e-ph coupling effects of the half-breathing Cu-O bond stretching mode, the inclusion of a screened on-site Coulomb interaction (U) in the LSDA+U calculations greatly enhances the e-ph coupling strength of this mode. The full breathing mode, on the other hand, shows a much weaker e-ph renormalization effect. Enhanced oxygen-$\rho$ character of the top valence states, together with the (local) antiferromagnetic spin ordering, seems to be responsible for a strong e-ph coupling of the half-breathing mode in the LSDA+U calculations.

3:42PM L8.00008 “Underlying Fermi surface” and violation of Luttinger count in strongly correlated superconductors, MOHIT RANDERIA, RAJDEEP SENSARMA, NANDINI TRIVEDI, The Ohio State University — The question of determining the “underlying Fermi surface” (FS) that is gapped out by superconductivity (SC) is of great importance in strongly correlated systems, particularly in view of angle-resolved photoemission (ARPES) experiments. We explore various definitions for the FS in the T=0 SC state using the zero-energy Green’s function, the excitation spectrum and the momentum distribution. We examine (i) the d-wave SC in high Tc cuprates, and (ii) the s-wave superfluid in the BCS-BEC crossover. In each case we show [1] that the various definitions agree, to a large extent, but all of them violate the Luttinger sum rule and do not enclose the total electron density. We discuss the important role of chemical potential renormalization and incoherent spectral weight in this violation. We show that the magnitude of the violation scales like $(\Delta/E_F)^2$, and its sign correlates with the electron-like or hole-like topology of the FS. These results are in good agreement with ARPES data on LSSCO [2].

4:06PM L8.00009 High Energy features in the photoemission spectra of cuprates. Arkady Shekhter, Chandra Varma, University of California, Riverside — We calculate the real part of the self-energy of fermions scattering off the quantum critical fluctuations derived for cuprates. At the upper cut-off of the quantum critical fluctuation spectra a logarithmic divergence in the real part of the self-energy occurs. The position of the peak of the one-particle spectral function is pinned near this divergence. This explains the high energy features observed in angle-resolved photoemission in cuprates superconductors.

4:18PM L8.00010 The nature of the two energy scales in underdoped superconducting cuprates1, Elena Bascones, Belen Valenzuela, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC) — Raman and ARPES experiments have demonstrated that in superconducting underdoped cuprates nodal and antinodal regions are characterized by two energy scales instead of the one expected in BCS. Using the Yang, Rice and Zhang (YRZ) model, in which pseudogap and superconductivity compete below a critical doping, we find that the antinodal Raman pair-breaking peak shifts to higher frequency with underdoping, follows the antinodal ARPES gap and is closely connected with the pseudogap. Its intensity decreases due to the competition between pseudogap and superconductivity. The nodal scale follows the doping dependence of the superconducting order parameter (cond-mat/0611154).

1 Financial Support from CSIC and CAM through grant 200500M136 is acknowledged

4:30PM L8.00011 “String excitations” of a hole in a quantum antiferromagnet and ARPES data. Efstratios Manousakis, Physics Department, Florida State University, USA, and Physics Department, University of Athens, Greece — Currently, high resolution angle-resolved photoelectron spectra (ARPES) from cuprates have been reported where an anomalous high-energy dispersion was identified. We suggest that these ARPES results reveal the internal structure of the hole quasiparticle in quantum antiferromagnets and more importantly it is evidence for the existence of “string-excitations” which validate early predictions based on the t-J model and related models. The following features of the ARPES results are all in agreement with predictions without adjusting any parameters: (a) the energy-momentum dispersion of the string-excitations, (b) the manner in which the spectral weight is transferred to higher energy string excitations, and (c) the vanishing of the quasiparticle spectral weight near the Γ point.

4:42PM L8.00012 Doping dependence of quasi-particle gaps at low hole doping in the Hubbard model.1, Markus Aichhorn, University of Wurzburg, Enrico Arrigoni, University of Technology Graz, Michael Potthoff, Werner Hanke, University of Wurzburg — Using the variational cluster approach we investigate the doping dependence of the pseudogap and the superconducting gap in the t′-t′′-t′′′ Hubbard model at low hole doping and zero temperature. The self energy of the system is calculated on a well suitable reference system for the investigated doping range and provides well defined quasi particles in the nodal region. We show that the pseudogap in the paramagnetic regime decreases with increasing hole doping, whereas the superconducting gap in the superconducting solution shows the opposite doping dependence for low hole doping. Furthermore our calculations suggest that the superconducting pseudogap in the antinodal region can be seen as sort of superposition of the paramagnetic pseudogap and the superconducting gap as measured near the nodal region. Thus, we claim that the occurrence of two distinct energy gaps recently found in experiments can naturally be explained by the single-band Hubbard model.

1Supported by DFG research unit FOR 538

4:54PM L8.00013 Dynamic mean field theory of the Gutzwiller-projected BCS Hamiltonian: phase fluctuation and pseudogap. Kwon Park, Korea Institute for Advanced Study — One of the most prominent problems in high temperature superconductivity is the nature of the pseudogap phase in the underdoped regime and its relationship to phase fluctuations. In this context, the Gutzwiller-projected BCS Hamiltonian is a useful model especially suited for the study of high temperature superconductivity in the underdoped regime due to the fact that there is an exact mapping to the Heisenberg model at half filling and a close connection to the t-J model at low doping in general. To be concrete, we have developed a dynamic mean field theory of the d-wave BCS Hamiltonian with on-site repulsion U. The large U limit corresponds to the Gutzwiller-projected BCS Hamiltonian. Effects of the phase fluctuations are studied as a function of on-site repulsion U and doping χ.

5:06PM L8.00014 Dynamical Cluster Approximation results for the effect of long range hoppings on Tc in Cuprates. Ehsan Khatami, Alexandru Macridin, Mark Jarrell, University of Cincinnati — The Dynamical Cluster Approximation along with the Quantum Monte Carlo (QMC) algorithm are employed to study the effect of long-range hoppings on the superconducting critical temperature of Cuprates. A two-dimensional t-t′-t′′-U Hamiltonian describes the physics of copper oxide planes in this model. We perform calculations on 4-site and 16-site clusters. The results show a weak dependence of the maximum Tc on the long-range hoppings. We see a suppression of Tc due to t′ in the hole-doped systems. t′ increases the critical doping (the doping beyond which the superconducting phase disappears) in the hole-doped regime, but this doping value is decreased by including t′′.

5:18PM L8.00015 Impurity Induced Kondo-like Screening in Cuprates. Wei Chen, Department of Physics, University of Florida, PO Box 118440, Gainesville, FL 32611, USA, Marc Gabay, Laboratoire de Physique des Solides, Université Paris-Sud, 91405 Orsay, France, Peter J. Hirschfeld, Department of Physics, University of Florida, PO Box 118440, Gainesville, FL 32611, USA — We study the magnetic response of t-t′-t′′-J model to a single nonmagnetic impurity using slave boson mean field theory, with restricted Bogoliubov-de-Gennes (BGD) method which allows us to deal with the strong correlations and reduction of order parameters around the impurity self-consistently. The temperature dependence of the paramagnetic susceptibility χ follows a Kondo-like form 1/(T + Θ), where the screening temperature increases with increasing doping. Both this form and the magnitude of χ are consistent with NMR experiments in the normal state of Zn doped YBCO.

Tuesday, March 6, 2007 2:30PM - 5:30PM –
Session L9 DCMP: Superconducting Fluctuations  Colorado Convention Center Korbel 1D
LERIDON, CNRS/ESPCI, 10 rue Vauquelin, 75005 Paris (France), JOHAN VANACKEN

1 debated and the answer to this question turns out to be essential for the understanding of high-$T_c$ superconductivity. One doesn’t know if the pseudogap is related to superconductivity or to an order in competition. In the former case, it has been suggested that superconducting pairing fluctuations may be responsible for the partial suppression of electronic excitations. This remains to be tested experimentally, but most of the probes used to investigate the pseudogap are not sensitive to pairs and therefore cannot provide such a test. Here, we report for the first time on a direct test of pairing fluctuations in the pseudogap regime using a Josephson-like experiment. Our results shows that fluctuations survive only in a restricted range of temperature close to $T_c$ ($T_c - T < 15K$), and therefore cannot be responsible for the opening of the pseudogap at high temperature.

2:42PM L9.00002 Evidence for Quantum Criticality (QC) and Universal Field-Induced Quantum Fluctuations (QF) in Cuprate Superconductivity (SC)1. H. YANG, A.D. BEYER, Physics Dept., Caltech, Pasadena, CA, V.S. ZAPF, NHHMF-LANL, Los Alamos, NM, M.S. PARK, K.H. KIM, S.-I. LEE, Physics Dept., Pohang University, Korea, N.-C. YEH, Physics Dept., Caltech, Pasadena, CA — We present experimental evidence for universal field-induced QF among cuprate superconductors as the result of their proximity to QC and the coexistence of SC and competing orders. We employ various experimental techniques to derive the in-plane magnetic irreversibility field in hole- and electron-type cuprate superconductors of varying doping levels and numbers of CuO$_2$ layers per unit cell, and we find strong suppression of the extrapolated zero-temperature in-plane irreversibility field relative to the paramagnetic field in all cuprates, suggesting universal field-induced QF. The irreversibility fields follow a universal dependence on a parameter that combines the effect of the doping level, electronic anisotropy, and charge imbalance in multi-layer samples.

2:54PM L9.00003 Magnetic field effect on the superconductivity fluctuation of cuprates, LSCO and LCCO measured by microwave broadband technique, A. MAEDA, T. OHASHI, Dept. Basic Sci., Univ. Tokyo, H. KITANO, Dept. Basic Sci., Univ. Tokyo, L. GOMEZ, CREST, JST, and Dept. Basic. Sci., Univ. Tokyo, I. TSUKAKA, CRIEPI, A. TSUKADA, M. NAITO, Dept. Appl. Phys., Tokyo Univ. Agriculture and Tech. — Understanding of the electronic phase diagram is essential to clarify the mechanism of high-$T_c$ superconductivity (SC) of cuprates. Previously, we studied the SC fluctuation of hole doped LSCO by microwave broadband technique, and found that there was a sharp crossover from the 2D-XY (BKT) behavior to the 3D-XY behavior by changing the doping. However, behaviors in the overdoped region and the effect of disorder were remained to be seen as future issues. To answer these, we investigated the effect of magnetic field on the SC fluctuation on LSCO with various carrier concentrations. For underdoped samples, the BKT behavior observed in zero-field experiments survived. However, the divergence of correlation length was found to be suppressed by the externally applied magnetic field. In contrast, for optimally doped samples, the range of the 3D-XY behavior became narrowed definitively under finite magnetic field. These provide strong support for our previous conclusion that there is a sharp change in the SC nature around at the optimum doping. The data in the overdoped LSCO and in electron doped cuprate LCCO will also be presented in a comparative manner.

3:06PM L9.00004 Superconducting fluctuations in underdoped $La_{2-x}Sr_xCuO_4$ thin films, BRIGITTE LERIDON, CNRS/ESPCI, 10 rue Vauquelin, 75005 Paris, France, JOHAN VANACKEN1, TOM WAMBECQ, VICTOR MOSHCHALKOV, INPAC, KU Leuven, Celestijnenlaan 200 D, B-3001 Heverlee, Belgium — Underdoped $La_{2-x}Sr_xCuO_4$ thin films resistivity was measured under high pulsed magnetic fields (50 T) in order to suppress superconductivity and extract the paraconductivity, or the conductivity due to superconducting fluctuations. Quite surprisingly, this paraconductivity is consistent without any adjustable parameter with a Gaussian model for the fluctuations, where both amplitude and phase of the order parameter fluctuate, as calculated by Aslamazov and Larkin (AL). This tends to indicate that the pairs responsible for the transition at $T_c$ are not preformed, as that would rather lead to Kosterlitz-Thouless type fluctuations. At higher temperature, the paraconductivity departs from AL behavior and follows a power law in $1/T$. At intermediate magnetic fields, the possibility of a quantum superconductor/insulator phase transition is investigated, as a plateau in the resistance versus temperature is observed under perpendicular magnetic field for all underdoped films.

3:18PM L9.00005 Determination of the dynamical scaling exponent in the superconducting to normal metal phase transition1, HUA XU, SU LI, CHRIS LOBB, STEVEN ANLAGE, Center for Superconductivity Research, Department of Physics, University of Maryland, College Park, MD 20742-4111 — In the high Tc superconductors, measurements of fluctuation effects reveal interesting behavior. Thermodynamic measurements have been done to investigate scaling behavior, to obtain critical exponents and to test the universality of the transition and the 3D XY model. Transport measurements of critical fluctuations, such as the AC conductivity, are less explored, and a wide range of critical exponents have been reported. We have investigated critical fluctuations in the microwave conductivity of YBa$_2$Cu$_3$O$_{7-δ}$ films. Our improved temperature stability and conductivity calibration(10 MHz to 50 GHz) allow us to take high quality data at small temperature intervals(50mK). This improves the conventional data analysis method and allows a new method of extracting exponents to be developed. With these two methods, we determined consistent values of $T_c$ and the critical exponent using eight different samples.

3:30PM L9.00006 Superconducting fluctuations and disorder in high-Tc cuprates, FLORENCE RULLIER-ALBENQUE, CEA, Saclay, France, HENRI ALLOUL, CNRS, LPS, Univ.Orsay, France, CYRIL PROUST, LINCM, Toulouse, France — The determination of critical fields and of the superconducting fluctuations in the cuprates are still highly debated questions, as both extremely high field and reduced $T_c$ cuprates are required to attempt to reach the normal state regime. We have studied in fields up to 60T the variation of the transverse magnetoresistance (MR) of underdoped YBCO crystals either pure or with $T_c$ reduced down to 3.5K by electron irradiation [1]. We show that the normal state MR is restored above a threshold field $H_c(T)$, which is found to vanish at $T_c' >> T_c$. This allows us to evidence a $(H,T)$ range where superconductivity survives at least as fluctuations. When $T_c$ is decreased by disorder, we found that the fluctuation range expands significantly as $T_c'$ is slightly depressed. This $T_c'$ behaves similarly versus defect content as the onset temperature $T_c$ of the Nernst signals measured on the same samples [2] which indicates that the $T_c$ decrease is partly due to the loss of the phase coherence. We found that $H_c'(T)$ and $T_c'$ which can be related to pair formation are depressed, although moderately, by the introduction of defects in contrast to the pseudogap temperature which is known to be insensitive to disorder, showing that these energy scales are not related.

Kosterlitz-Thouless transition was directly related to the biasing current as well as temperature. The duration of the voltage pulses depended on the device geometry (with the high-kinetic inductance meander structures having longer, nanosecond, pulses) while their rate thermal fluctuations break them apart causing the order parameter to momentarily reduce to zero, which in turn causes a transient voltage pulse. The duration of the Kosterlitz-Thouless-type fluctuations, where the high enough applied bias current reduces the binding energy of vortex-antivortex pairs and, subsequently, we have observed fluctuations, manifested as sub-nanosecond to nanosecond transient, millivolt-amplitude voltage pulses, generated in two-dimensional NbN films.

We believe they are due to the thermal activated phase slips. The frequency dependence of the fluctuations suggests the observation of the ac Josephson effect above $T_c$.

Conducting Films, PAUL ORETO, STEVEN KIVELSON, Department of Physics, Stanford University, BORIS SPIVAK, Department of Physics, University of Washington, Seattle — Treating the inhomogeneous solution of the BCS mean-field equations as the saddle point of an effective quantum action, we derive the theory of the superconductor to metal transition in films under the conditions in which the critical resistance is small compared to the quantum of resistance. The present results are applicable to the magnetic field driven transition in MoGe films. It is also applicable to the transition in zero field in a weakly coupled d-wave superconductor, which may in turn be a useful caricature of a cuprate high temperature superconductor.

Fluctuations and Glassy Behavior in the 2D Superconductor-Insulator Transition in Granular Bismuth1. KEVIN PARENO, SARWA TAN, ALLEN GOLDMAN, University of Minnesota — The superconductor-insulator transition has been investigated in granular, amorphous bismuth films. The system's dynamics have been investigated at various levels of disorder by incrementing film thickness and measuring voltage fluctuations. In insulating films in which local superconductivity was not evident, the first power spectra had $1/f^2$ frequency dependences. In films that exhibited local superconductivity, the spectra had weaker frequency dependences. In a film with low enough disorder, the resistance had a very weak temperature dependence below 1.5 K and non-ergodic behavior and strong fluctuations were observed below 400 mK. The variations of the first and second power spectra with disorder and temperature will be discussed.

This work was supported by the National Science Foundation under grant no. NSF/DMR-045121.

The approach to a superconductor-to-Bose-insulator transition in disordered films, NICHOLAS P. BREZNAY, M. A. STEINER, A. KAPITULNIK, Stanford University — We study the superconductor-insulator transition in the limit of strongly disordered films of indium oxide. It was observed previously that the insulating phase is strengthened as the disorder increases, creating a strong barrier to pair-breaking in the vicinity of the critical point. We find that for the strongest insulators, the critical resistance is approximately the universal resistance for pairs, $R_Q = \hbar/4e^2$ and the scaling of both the linear and non-linear resistance is consistent with the quantum percolation solution to the dirty boson model. We combine these results with previous data and note separate branches corresponding to strong and weak disorder. The strong disorder branch suggests a true dirty boson superconductor-insulator transition.

Observation of Pairing Correlations in Strongly Localized Amorphous Films, M.D. STEWART, JR., J.M. VALLES, JR., AJIJUN YIN, J.M. XU, Brown University — We have measured the Superconductor to Insulator Transition (SIT) as a function of thickness at dilution refrigerator temperatures in ultrathin Bi/Sb films perforated with a regular honeycomb array of holes separated by 100 nm. The presence of these perforations profoundly influences the character of the transition. In particular, on the insulating side of the SIT, the resistance as a function of temperature, $R(T)$, rises monotonically and becomes activated below 1K. Closer to the SIT, a minimum develops in the $R(T)$ suggesting of strong superconducting fluctuations and the onset of Cooper pairing. Simultaneously, the perpendicular field magnetoresistance begins to oscillate with a period that corresponds to the superconducting flux quantum. Yet thicker films exhibit a relatively broad $R(T)$ transition toward a zero resistance state. This behavior constitutes direct evidence that the superconducting ground state of this amorphous film system emerges from an insulating state containing localized Cooper pairs.

This work has been supported by the NSF through DMR-0203608, and DMR-0605797, AFRL, and ONR.

Nonequilibrium Voltage Fluctuations in Aluminum Wires, M. REZNIKOV, A. FRYDMAN, M. REESE, D. PROBER, Technion, Israel Institute of Technology — We present measurements of the nonequilibrium voltage fluctuations across current biased superconductive aluminum wires in the vicinity of $T_c$. Above $T_c$, these voltage fluctuations are due to superconductive fluctuations which persist on the time scale of the Ginzburg time. Below $T_c$ we believe they are due to the thermal activated phase slips. The frequency dependence of the fluctuations suggests the occurrence of the ac Josephson effect above $T_c$.

Fluctuations in Two-Dimensional Superconducting NbN Nanobridges and Nanostructures Meanders, JENNIFER KITAYGORSKY, I. KOMISSAROV, A. JUKNA, University of Rochester, O. MINAEVA, N. KAuroVA, A. DIVOCHY, A. KORNEEV, M. TARKHOV, B. VORONOV, I. MILOSTNAYA, G. GOL'TSMAN, Moscow State Pedagogical University, R. SOBOLEWSKI — We have observed fluctuations, manifested as sub-nanosecond to nanosecond transient, millivolt-amplitude voltage pulses, generated in two-dimensional NbN nanobridges, as well as in extended superconducting meander nanostructures, designed for single photon counting. Both nanobridges and nano-stripe meanders were biased at currents close to the critical current and measured in a range of temperatures from 1.5 to 8 K. During the tests, the devices were blocked from all incoming radiation by a metallic enclosure and shielded from any external magnetic fields. We attribute the observed spontaneous voltage pulses to the Kosterlitz-Thouless-type fluctuations, where the high enough applied bias current reduces the binding energy of vortex-antivortex pairs and, subsequently, thermal fluctuations break them apart causing the order parameter to momentarily reduce to zero, which in turn causes a transient voltage pulse. The duration of the voltage pulses depended on the device geometry (with the high-kinetic inductance meander structures having longer, nanosecond, pulses) while their rate was directly related to the biasing current as well as temperature.

Interaction of vortices in thin superconducting films and Berezinskii-Kosterlitz-Thouless transition1. VLADIMIR KOGAN, Ames Lab — The precondition for the BKT transition in thin superconducting films, the logarithmic intervortex interaction, is satisfied at distances short relative to $\Lambda = 2\pi^2/d$, $\lambda$ is the London penetration depth of the bulk material and $d$ is the film thickness. For this reason, the search for the transition has been conducted in samples of the size $L < \lambda$. It is argued below that film edges turn the interaction into near exponential (short-range) thus making the BKT transition impossible. If however the substrate is superconducting and separated from the film by an insulated layer, the logarithmic intervortex interaction is recovered and the BKT transition should be observable.

Density of States, Entropy, and the Superconducting Pomeranchuk Effect in Pauli-Limited Al Films, GIANLUIGI CATELANI, Laboratory of Atomic and Solid State Physics, Cornell University, XIAOSONG WU, PHILIP ADAMS, Department of Physics and Astronomy, Louisiana State University — We present low temperature tunneling density of states measurements of Pauli-limited Al films in which the Zeeman and orbital contributions to the critical field are comparable. We show that films in the thickness range of 6-7 nm exhibit a reentrant parallel critical field transition which is associated with a high entropy superconducting phase, similar to the high entropy solid phase of $^3$He responsible for the Pomeranchuk effect. This phase is characterized by an excess of states near the Fermi energy so long as the parallel critical field transition remains second order. Theoretical fits to the zero bias tunneling conductance are in good agreement with the data well below the transition but theory deviates significantly near the transition. The discrepancy is a consequence of the emergence of the $e-e$ interaction correlations as one enters the normal state.
Tuesday, March 6, 2007 2:30PM - 4:54PM –
Session L10 DCMP: Heavy Fermions in the 115 Compounds  Colorado Convention Center Korbel 1E

2:30PM L10.00001 Incoherent Non-Fermi Liquid Scattering in a Kondo Lattice. JOHNPIERRE PAGLIONE, T.A. SAYLES, P.-C. HO, M.B. MAPLE, Department of Physics, University of California, San Diego — The effect of Kondo lattice dilution was investigated in the heavy-fermion superconductor CeCoIn$_5$ to study the evolution of unconventional superconductivity and non-Fermi liquid properties. A systematic substitution of both non-magnetic (full or empty $f$-shell) and large, stable $f$-moment rare earth impurities into high-quality single-crystal specimens of Ce$_{1-x}$R$_x$CoIn$_5$ (where R=Y, Pr, Gd, Er and Lu) has revealed two contrasting features. First, both superconducting electron pair-breaking and the suppression of Kondo coherence proceed in a manner which is insensitive to the magnetic state of the dopant atom, suggesting spin-independent disorder is the dominant perturbation in both phenomena. In contrast, the evolution of the non-Fermi liquid properties with substitution shows a striking sensitivity to the dopant atom’s $f$-moment configuration.

$^1$Research supported by the US DOE (DE-FG02-004ER-046105), NSF (DMR-03-35173) and NSERC of Canada.

2:42PM L10.00002 Effects of self-irradiation on local crystal structure and 5$f$ localization in PuCoGa$_5$. C. H. BOOTH, M. DANIEL, R. E. WILSON, Lawrence Berkeley National Laboratory, E. D. BAUER, J. N. MITCHELL, N. O. MORENO, L. A. MORALES, J. L. SARRAO, Los Alamos National Laboratory, P. G. ALLEN, Lawrence Livermore National Laboratory — X-ray absorption fine-structure (XAFS) measurements demonstrate the structural and electronic changes involved in destroying superconductivity in PuCoGa$_5$ due to self-irradiation damage. In particular, the Pu $L_{III}$-edge data indicate a more localized 5$f$-orbital relative to the itinerant paramagnet UCoGa$_5$, potentially increasing with radiation damage. Moreover, the local crystal structure in aged material is disordered much more strongly than expected, consistent with all atoms within a damage cascade displaced from their equilibrium positions.

2:54PM L10.00003 Superconductivity due to cooperative two-channel Kondo effect. MAXIM DZERO, KASTURI BASU, PIERS COLEMAN, Rutgers University — We discuss the application of the co-operative two-channel Kondo model to describe the low temperature properties of the Ce and Pu based 115’s. Based on the crystal field multiplet structure for Ce and Pu ions in tetragonal symmetry, we employ the group theory to justify the validity of the two-channel Kondo physics. Additional screening channel contributes to destabilization of the Fermi liquid and leads to development of the heavy Fermi surface. The fluctuations between the zero modes for the Kondo singlets leads to divergent composite pair susceptibility.

3:06PM L10.00004 Coexistence of antiferromagnetism and superconductivity in a model for CeRhIn$_5$. JOSE V. ALVAREZ, Universidad Autonoma de Madrid, Spain, FELIX YNDURAIN, Universidad Autonoma de Madrid, Spain — The finite temperature phase diagram of CeRhIn$_5$ as a function of pressure and magnetic field has three main highlights: 1) the competitive coexistence of metallic antiferromagnetism and superconductivity, 2) the abrupt disappearance of antiferromagnetism when the Neel and superconducting temperatures become equal at a critical pressure $P_c$, and 3) the reentrance of the antiferromagnetic phase in a range of pressures larger than $P_c$ when a magnetic field is applied. Based on first-principles band structure calculations, we propose a quasi-two-dimensional model of interacting electrons, which reproduces, at the mean-field level, the central features of the phase diagram. We also discuss the divergence of the cyclotron mass observed in dHvA oscillations and the amount entropy released at the orderings temperatures.

3:18PM L10.00005 Quantum Criticality in Cd doped CeMIn$_5$. FILIP RONNING, YOSHI TOKIWA, JOE THOMPSON, ROMAN MOVSCHOVICH, Los Alamos National Lab, LONG PHAM, UC Davis, ZACHARY FISK, UC Irvine — In pure CeMIn$_5$, the application of magnetic field has revealed a field tuned quantum critical point surprisingly coincident with the superconducting $H_{c2}$. The application of pressure suppressed the antiferromagnetic fluctuations in the system and pushed the quantum critical field inside the superconducting dome. By substituting Cd for In it was shown that one can quickly induce the antiferromagnetic state. With predominantly thermodynamic probes, such as specific heat, we investigate how the appearance of long range antiferomagnetic order induced by Cd doping influences the field tuned quantum critical behavior. This will also be contrasted with the behavior found for the antiferromagnetic quantum critical point seen in CeRhIn$_5$, under pressure.

$^1$Work at LANL was performed under the auspices of US DOE. We also acknowledge NSF-DMR-0503360 for support.

3:30PM L10.00006 Multiple vortex phases in the heavy fermion superconductor CeCoIn$_5$. A. D. BIANCHI, Z. FISK, Dept. Phys. & Astro., UC Irvine, Irvine, CA, USA, M. KENZELMANN, J. MESOT, J. KOHLBRECHER, M. ZOLLIKER, LNS, PSI & ETHZ, Switzerland, L. DEBEER-SCHMITT, M. R. Eskildsen, Dept. of Physics, University of Notre Dame, Notre Dame, IN, USA, J. S. WHITE, E. M. FORGAN, School of Phys. and Astro., U. of Birmingham, Birmingham, UK, E. D. BAUER, J. L. SARRAOD, MPA-10, LANL, Los Alamos, NM, USA, C. PETROVIC, Cond. Matt. Phys., BNL, Upton, NY 11793, USA — We report the entire HT-phase diagram of the vortex lattice (VL) in CeCoIn$_5$ for fields applied along the crystallographic c-axis. At the upper critical field $H_{c2}$ of about 5 T and 50 mK, we observe a distorted hexagonal flux lattice, which first gives way to a rhombic lattice at 4.3 T and then to a square lattice at 3.3 T, before entering the previously reported flux lattices at lower fields. The distorted hexagonal phase extends to lower fields and higher temperatures than the $H_{c2}$-phase space that was previously assigned to a inhomogeneous FFLO state by magnetization and NMR measurements. Surprisingly, we also observed an increase of the flux lattice form factor as a function of increasing field in the rhombic phase, in contrast to the flux lattice in most superconductors. We will discuss the relevance of these results for the presence of the FFLO and magnetic phases.

3:42PM L10.00007 Nature of a possible FFLO state in CeCoIn$_5$ as revealed by NMR. GEORGOS KOUTROULAKIS, VESNA MITROVIC, MARC-ANDRE VACHON, Brown University, Providence, RI, MLADEN HORVATIC, CLAUDE BERTHIER, GHMFL, Grenoble, France, GEORG KNEBEL, GERARD LAPERTOT, JACQUES FLOQUET, SPSMS, CEA, Grenoble, France — We report low temperature $^{115}$In nuclear magnetic resonance (NMR) measurements of the heavy-fermion superconductor CeCoIn$_5$ in high magnetic fields. We will discuss the implications of our findings for the nature of a possible inhomogeneous superconducting state, the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state, in this compound.

3:54PM L10.00008 Superconductivity and magnetism in heavy-fermion systems. DANIEL E. SHEEHY, JOERG SCHMALIAN, Ames Lab and Iowa State University — Recent experiments on CeCoIn$_5$ have observed coexisting superconductivity and magnetic order under an applied magnetic field near the Pauli limit. Motivated by such observations, we study the interplay between pairing and magnetism in the SU(N) Kondo lattice model, believed to provide an accurate description at low temperatures of such heavy-fermion systems. We present results for the phase diagram as a function of temperature and magnetic field.
4:06PM L10.00009 Effect of pressure on hole-doped CeCoIn$_5$ and CeRhIn$_5$. V. A. SIDOROV, TUSON PARK, J. D. THOMPSON, Los Alamos National Lab, L. D. PHAM, S. MAQUILON, U. C. Davis, Z. FISK, U. C. Irvine — With one less $p$-electron than In, Cd or Hg adds one hole per substituted In in CeMIn$_5$ ($M$=Co,Rh, Ir). Progressive Cd/Hg substitutions tune the ground state of superconducting CeCoIn$_5$ to one of coexisting magnetism and superconductivity and eventually to antiferromagnetic only. This systematic evolution of states in doped CeCoIn$_5$ is reversed accurately by applied pressure and maps onto the temperature-pressure phase diagram of pure CeRhIn$_5$. These observations, together with the response of Cd-substituted CeRhIn$_5$ to applied pressure, show that ground states of CeMIn$_5$ are controlled by fine details of electronic structure and that disorder on the In site and different ionic radii of Cd and Hg have an insignificant effect.

1ZF, LDP and SM acknowledge support by NSF-DMR-0503360. Work at Los Alamos was performed under the auspices of the US DOE, Office of Science.

4:18PM L10.00010 Magnetic and electrical transport properties of Ce$_{1-x}$Nd$_x$CoIn$_5$. CEDOMIR PETROVIC, Condensed Matter Physics, Brookhaven National Laboratory, Upton NY 11973, JACOB HUDIS, Department of Physics and Astronomy, Johns Hopkins University, Baltimore MD 21218, RONGWEI HU, Condensed Matter Physics, Brookhaven National Laboratory, Upton NY 11973, YONGJAE LEE, Department of Earth System Sciences, Yonsei University, Seoul 120749 Korea, VESNA MITROVIC, Physics Department, Brown University, Providence RI 02912, COLLIN BROHOLM, Department of Physics and Astronomy, Johns Hopkins University, Baltimore MD 21218 — Single crystals of Ce$_{1-x}$Nd$_x$CoIn$_5$ ($0 \leq x \leq 1$) were grown by molten metallic flux technique. Synchrotron powder X-ray diffraction confirms phase purity and smooth evolution of the lattice parameters with increased Nd concentration. Evolution of the ground state in this alloy series between heavy fermion superconducting for $x = 0$ (CeCoIn$_5$) and antiferromagnetic for $x = 1$ (NdCoIn$_5$) will be presented.

4:30PM L10.00011 In-plane torque measurements on CeCoIn$_5$ single crystals. H. XIAO, T. HU, C.C. ALMASAN, Kent State University, Kent, Ohio 44240, USA, T.A. SAYLES, M.B. MAPLE, University of California at San Diego, La Jolla, California, 92903, USA — In-plane torque measurements were performed on single crystals of CeCoIn$_5$ in the mixed state in order to determine the symmetry of the superconducting gap. The reversible part of the mixed state torque shows a four fold symmetry. The sign of the four fold symmetry is positive. The amplitude of the in-plane torque first increases with increasing magnetic field $H$, and then decreases with further increasing field until it vanishes towards $H = 0$. Sharp irreversible peaks are present in the irreversible torque at 45, 135, 225, and 315°. These experimental results imply d$_{x^2-y^2}$ symmetry of the superconducting order parameter. We also performed in-plane torque measurements in the normal state. Another four fold symmetry is found which has a different origin than the one in the mixed state. The amplitude of the normal state torque has an $H^4$ dependence and it shows no saturation up to 14 T. This later four fold symmetry could be related with the symmetry of the Fermi surface.

1This research was supported by the National Science Foundation under Grant No. DMR-0406471 at KSU and the US Department of Energy under Grant No. DE-FG02-04ER46105 at UCSD.

4:42PM L10.00012 Flux Growth of Heavy Fermion LiV$_2$O$_4$ Single Crystals. S. DAS, X. ZONG, A. NIAZI, D.C. JOHNSTON, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, IA 50011 — The spinel-structure compound LiV$_2$O$_4$ is a rare $d$-electron heavy fermion. Measurements on single crystals are needed to clarify the mechanism for the heavy fermion behavior. In addition, it is known that small concentrations (< 1 mol%) of magnetic defects in the structure strongly affect the properties, and measurements on single crystals containing magnetic defects would help to understand the latter behaviors. Herein, we report growth at 950–1030 °C of 1 mm$^3$ octahedron-shaped LiV$_2$O$_4$ single crystals using a self-flux technique. The magnetic susceptibility of the as-grown crystals shows a Curie-like upturn at low temperatures arising from $\approx 0.5$ mol% magnetic defects within the spinel structure. After annealing at 700 °C, the Curie-like upturn (and magnetic defects) disappeared in some crystals, thus revealing the known intrinsic nearly temperature-independent behavior below ~20 K. Preliminary heat capacity measurements on as-grown crystals containing magnetic defects showed a high linear specific heat coefficient $\gamma = 450$ mJ/(mole K$^2$) at 1.8 K. Additional electronic transport, magnetic and thermal measurements on both as-grown and annealed crystals will be presented.

1Work supported by the USDOE under Contract No. W-7405-Eng-82.

Tuesday, March 6, 2007 2:30PM - 5:30PM –
Session L23 DCMP: High Pressure IV Colorado Convention Center 110

2:30PM L23.00001 On the high pressure behavior of body-centered cubic iron. FLORIN APOSTOL, SHEN QIU, PAUL MARCUS, Florida Atlantic University — The high pressure–high temperature behavior of iron is of current interest for geophysical reason, i.e., the earth’s core is believed to be iron at high p and T. The value of the pressure at which the rigid lattice of body-centered-cubic ferromagnetic iron goes unstable was recalculated by newer methods. We give some thermodynamic arguments in support of our procedure, which minimizes the Gibbs free energy at constant pressure rather than internal energy at constant volume, and then finds elastic constants as second derivatives of G with respect to strains. The calculations used WIEN2k band-structure program and a minimum path program that makes a series of jumps in structure based on the local slope and curvature of G at a point in structure space. Errors are pointed out in several recent papers that found values different than ours, mainly due to neglect of the pressure correction required when elastic constants are calculated in a system under finite pressure by differentiation of the energy rather than Gibbs free energy.

2:42PM L23.00002 Rheology under conditions of the Earth’s inner core. ANATOLY BLOMONSHKO, Applied Materials Physics, Institutes of Materials Science & Engineering and Theoretical Physics, The Royal Inst. of Technology, 10044 Stockholm, SE — It is well established that the solid Earth’s inner core (IC) consists of an iron-rich alloy. However, low rigidity of the IC (Poisson ratio of about 0.44) remains enigmatic. Both measured at low temperature elastic properties of hexagonal (hcp) iron phase as well as the calculated properties of the various hypothetical iron phases at high pressure (above 3 Mbar) and high temperature (from 5000 to 8000 K) are inconsistent with seismological observations. The velocity of shear waves propagation in the IC is considerably lower than the measured/calculated shear velocity of iron phases. We performed ab initio as well as classical molecular dynamics (MD) simulations of iron polycrystals, grown from melt as well as obtained by the Voronoi construction. We demonstrate, that the account for grain boundaries and/or various structural inhomogeneities allow to bring the calculated data in close agreement with the experimental seismic data.
MOBERLY CHAN, JAMES MC NANEY, JAMES HAW RELI A K, HECTOR LOREN ZA NA, Lawrence Livermore National Laboratory — Time resolved, in-situ applied to examine the influence of the magnetic fluctuations on the free energy and thermal equation of state properties of bcc Fe at high temperatures. This Curie temperature, magnetization curve, and other finite-temperature magnetic properties through extensive Monte Carlo simulations, which have been further applied to shock the magnetic properties of bcc Fe at high temperatures. This work was supported by US Department of Energy ASCI ASAP subcontract to Caltech, Grant DOE W-7405-ENG-48.

3:06PM L23.0006 Multi-scale modeling of ferromagnetism in bcc Fe as a function of pressure and temperature. XIANWEI SHA, R. E. COHEN, Carnegie Institution of Washington — We investigate the magnetic properties of bcc Fe as functions of pressure and temperature using multi-scale modeling techniques. We employ a first-principles fitted tight-binding total-energy model in the generalized-gradient approximation to examine bcc Fe at numerous ferromagnetic, antiferromagnetic and spin spiral states, and fit the tight-binding data to a generalized Heisenberg Hamiltonian which includes both the on-site and local exchange energy to describe the magnetic energy for any arbitrary magnetic configuration. We obtain the Curie temperature, magnetization curve, and other finite-temperature magnetic properties through extensive Monte Carlo simulations, which have been further applied to shock the magnetic properties of bcc Fe at high temperatures. This work was supported by US Department of Energy ASCI ASAP subcontract to Caltech, Grant DOE W-7405-ENG-48 (to REC).

3:18PM L23.0005 Ellipsometry Measurements of Shock-Induced Phase Transitions. J. R. PATTERSON, J. H. NGUYEN, L. X. BENEDICT, J. E. KLEPEIS, N. C. HOLMES, Lawrence Livermore National Laboratory — In situ measurements of crystal structures and phase transitions during dynamic high-pressure experiments are complex, thus knowledge of high-pressure high-temperature phase diagrams for many materials is limited. Since typical Hugoniot EOS and sound speed experiments do not provide this information, we have developed an ellipsometric technique which allows the real-time measurement of optical constants. Coupling measured optical properties with calculations allows one to infer structural information complimentary to techniques such as x-ray diffraction. We present dynamic ellipsometry measurements of shock-induced solid-solid (α → Fe → ϵ → Fe) and solid-liquid (β → liquid − Sn) phase transitions. In addition, the time-resolution of such dynamic phenomena suggests that information on the kinetics of phase transitions as well as deformation/relaxation can be obtained. We will also discuss our efforts to incorporate multiple wavelengths into ellipsometry measurements of dynamically compressed materials.

3:30PM L23.0006 Symmetry breaking in a dense liquid: Why sodium melts at room temperature. Jean-Yves Raty, University of Liège, Belgium, Eric Schwegler, Lawrence Livermore National Laboratory, Stanimir Bonev, Dalhousie University, Canada — The melting curve of sodium measured in [1] exhibits unusual features under pressure: the melting temperature, Tm, reaches a maximum around 30 GPa followed by a sharp decline from 1000 K to 300 K in the pressure range from 30 to 120 GPa. In this study, the structural and electronic properties of molten sodium are studied using first principles theory. With increasing pressure, liquid sodium initially evolves by assuming a more compact local structure, which accounts for the maximum of Tm at 30 GPa. However, at pressure around 65 gigapascals a transition to a lower coordinated structure takes place, driven by the opening of a pseudogap at the Fermi level. Remarkably, the broken symmetry liquid phase emerges at rather elevated temperatures and above the stability region of a closed packed free electron-like metal. The theory explains the measured drop of the sodium melting temperature, down to 300 kelvin at 105 GPa. [1] Gregoryantz et al., Phys. Rev. Lett. 94, 185502 (2005).

3:42PM L23.0007 The breakdown of a simple-metal paradigm at high pressures, Bruno Rousseau, Neil W. Ashcroft, Cornell University — The light alkalis at one bar and room temperature are considered the paradigms of ‘simple-metal’ behavior. They adopt cubic structures and their valence bands are free electron-like. Under normal conditions this has been well accounted for by pseudopotential theory. It is a common expectation that the light alkalis might even be more free electron-like at higher densities, as impelled by pressure. Advances in diamond anvil cell methods have yielded new insights in the behavior of the alkalis at megabar pressures, presenting a considerable challenge to the above paradigm. Under pressure, the light alkalis adopt non-simple structures. Initial studies by Neaton and Ashcroft [Letters to Nature, Vol. 400, 141 (1999)] on lithium suggested that with increasing pressure the valence bands first broaden, but then start narrowing substantially. Corresponding to this, the valence charge density is localizing in the interstitial spaces of the lattice and the core bands are acquiring significant width. Our work focuses on showing that this behavior may be fairly general and can be explained at the one electron level as an emerging breakdown of the weak pseudopotential hypothesis.

3:54PM L23.0008 Melting of Sodium Under Pressure, Jan Vorberger, Ronald E. Cohen, Burkhard Militzer, Geophysical Laboratory, Carnegie Institution of Washington, Washington D.C., 20015 — The bcc, fcc, and liquid phases of sodium are investigated with density functional molecular dynamic (DFT-MD) simulations. We focus on the behavior of the melting curve at high pressure. Diamond anvil cell experiments have determined a melting line with a negative slope at pressures above 3GPa [1]. In the bcc phase, the melting temperature drops from around 1000K to 700K. It decreases even further to 300K in the fcc phase. We have performed simulations for sodium in a range from zero to 100 GPa, temperatures ranging from 300K to 2000K. Equations of State (EOS) for the bcc, fcc and liquid phase are obtained. To investigate the underlying principles of melting in sodium, we study ionic and electronic structure of solid and fluid. Using our EOS, we reproduce positive and negative slopes of the melting line in the proposed pressure regions for the bcc as well as for the fcc phase. [1] E. Gregorianz, O. Degtyarewa, M. Somayazulu, R.J. Hemley, H. Mao, Phys. Rev. Lett. 94, 185502 (2005)

E.S. worked under the auspices of the U.S. DoE at the University of California/LLNL under Contract No. W-7405-Eng-48.

1 This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

2 Work supported by the NSERC of Canada. J.Y.R. acknowledges support from the FNRS, the Nomade Region Wallonie contract and the FAME NoE. E.S. worked under the auspices of the U.S. DoE at the University of California/LLNL under Contract No. W-7405-Eng-48.
4:06PM L23.00009 An Investigation of s-d promotion at high pressure with the Projector Augmented Wave method. RYAN SNOW, University of California, Davis, JOHN PASK, Lawrence Livermore National Laboratory, CHING-YAO PONG, University of California, Davis — The PAW(L) method for ab initio density functional calculations combines advantages of both pseudopotential (PP) and all-electron (AE) methods. The PAW method provides accuracy comparable to AE methods, core-sensitive calculations, and ab initio molecular dynamics with large systems. The requirement for high accuracy in the determination of s-d promotion pressures in transition metals serves as a proving ground for the accuracy of the PAW method. We present PAW, PP, and AE APW+lo results for the case of Molybdenum, for which there is significant disagreement among recent ab initio predictions above 600 GPa. 1. P.E. Blochl, Physical Review B, 50, 17953 (1994)

1This work was performed, in part, under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory

4:18PM L23.00010 Quasi-Isentropic Compression of Ta Using Graded Density Impactors. J.R. PATTERSON, LLNL, J.H. NGUYEN, D.A. ORLIKOWSKI, R.W. MINICH, L.P. MARTIN, N.C. HOLMES — Recent advances in the fabrication of graded density impactors have enabled the production of smooth, continuous quasi-isentropes for gas gun experiments. Using these impactors, we have performed experiments on Ta in which the sample is initially shocked to 66 GPa on the Hugoniot and then quasi-isentropically compressed to over 1 Mbar. We will present the results of our simulations of the data and compare with previous Hugoniot measurements as well as the calculated isentrope of Ta. We will also discuss potential sources of error in both the data and analysis and their effect on the measured quasi-isentrope.

1This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

4:30PM L23.00011 A multi-scale, atomistic-based strength model for tantalum and molybdenum. DANIEL ORLIKOWSKI, Lawrence Livermore National Laboratory, LIN YANG, JOHN A. MORIARTY — For the description of bcc tantalum and molybdenum strength at the continuum level, there have combined several extensive sets of quantum-based, atomistic calculations into a new parameterization of the Steinberg-Lund (SL) and mechanical threshold stress (MTS) strength models. This model is then used to simulate recent gas-gun shock experiments. The atomistic calculations that determine the parameters of this model were derived from two disparate methods but both based on quantum-based generalized pseudopotential theory (MGPT) for the ion-ion interactions. In one method, Green’s function boundary conditions are used to relax dynamically the boundary forces in molecular dynamics simulations of the kink-pair activation enthalpy and Peierls stress for (a/2) < 111 > screw dislocations. The other method combines MGPT Monte Carlo simulations with full potential linear muffin-tin orbital (FP-LMTO) method of density functional theory to determine the temperature and pressure dependence of the shear modulus. We discuss the new parameterization of the models and hydrodynamic simulation results.

4:42PM L23.00012 Osmium under high pressure: a fully relativistic first-principles study of the structural and electronic properties. ALBERTO RUBIO-PONCE, Departamento de Ciencias Basicas, UAM-Azcapotzalco, Mexico., ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico — Recently, there has been much interest in the high-pressure properties of Os after that the first bulk modulus measurement was made only four years ago. It is important to mention that to date, the phase diagram of Os is unknown. In the present work, we have studied the structural and electronic properties of Os using the full-potential LAPW method and the GGA for the exchange-correlation functional. The calculations were performed including the spin-orbit coupling which is important for heavy metals like Os. The total-energy as a function of the cell volume was computed assuming the hcp, fcc, and ω structures, for compressions up to 65% of the equilibrium volume. In contradiction with the previous non-relativistic LDA-calculation, we find that Os in the hcp phase have lower energy than the fcc and ω structures. The hcp structure remains stable for pressures up to 400 GPa and not structural transition to the fcc or ω phase was found. Nevertheless, from the analysis of the band structure, we find an electronic topological transition induced by pressure at the high-symmetry point L, where three bands cross the Fermi level upon compression.

4:54PM L23.00013 Difference Frequency Generation Measurements of Phase Transitions in Gallium. MICHAEL FURLANETTO, Los Alamos National Laboratory — We recently measured the vibrational excitation spectra of solid and liquid gallium with ultrafast terahertz difference frequency generation (DFG) spectroscopy. The two phases had clearly different DFG spectra, with a 250 cm$^{-1}$ phonon feature visible in the solid phase and a 50 cm$^{-1}$ excitation feature seen in the liquid phase. Prospects for using this technique to measure phase transitions of shocked systems in situ will be discussed.

5:06PM L23.00014 First The motion and mobility of screw and edge dislocation in bcc tantalum. ROBERT RUDD, KYLE CASPERSEN, CHRISTINE WU, MEIJE TANG, Lawrence Livermore National Laboratory — Strength in bcc metals is, surprisingly, not well understood; it is thought to be dominated at low temperature by the motion of 1/2<111> screw dislocations. The mobility of these screw dislocations is thought to be controlled by nucleation and propagation of kinks along the dislocation line, which can at high stress result in the formation of debris (vacancies, interstitials, loops, etc) in the dislocation wake. We studied the motion of screw and edge dislocations in bcc tantalum by performing large-scale molecular-dynamics simulations using both Finnis-Sinclair potentials, and model-generalized-pseudopotential-theory (MGPT) potentials [1]. We present here simulation predications for dislocation motion, mobility, and debris formation with respect to pressure, temperature, and strain rate. [1] J. A. Moriarty, Phys. Rev. B 42, 1609 (1990); J. A. Moriarty, Phys. Rev. B 49, 12431 (1994).

1This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

5:18PM L23.00015 Material Strength on Quasi-isentropes. JEFFREY NGUYEN, Lawrence Livermore National Laboratory, JEREMY R. PATTERSON, DANIEL ORLIKOWSKI, LOUIS P. MARTIN, NEIL C. HOLMES, LAWRENCE LIVERMORE NATIONAL LABORATORY COLLABORATION — We have recently performed experiments to study strength properties of aluminum on quasi-isentropes. The aluminum samples were initially shocked to a fixed state on the Hugoniot, then quasi-isentropically compressed and released isentropically. In these experiments, the strain rates on compression and release areomers are nearly equal. We will discuss the details of the experiments and data and error analysis in deriving strength of aluminum. Recent advances in the functionally graded density impactor technology have made it possible for us to carry out these experiments with significantly reduced uncertainties. We will discuss these advances including reproducibility and planarity of the impactors. Methods to characterize these advances will be discussed. [1] Work performed under the auspices of the U.S. DOE at the University of California/Lawrence Livermore National Laboratory under contract W-7405-ENG-48.

Tuesday, March 6, 2007 2:30PM - 5:06PM – Session L27 DCMP: Glassy Systems Colorado Convention Center 301
2:30PM L27.00001 Pressure Dependence of the Glass-Transition Temperature for Intermediate and Fragile Glass-Forming Systems, WILLIAM OLIVER III, Physics Department, University of Arkansas, Fayetteville, AR 72701, ASHLEY ALTOM, HALEY BEVERBURG, JAMES COOPER III, DANIEL FROST, DAVID LEISCHKE, CHRISTOPHER WELLS — The glass transition temperature, $T_g$, is determined over the pressure range 0 to 80 kbar using a diamond anvil cell (DAC). Two methods are used: i) the onset or disappearance of pressure gradients indicated by ruby fluorescence, and ii) a new method in which $T_g(P)$ is determined by significant changes in slope in the P-T curve during pseudo-isobaric temperature ramps. This slope change accompanies the significant change in volume expansion coefficient between the highly viscous, metastable, supercooled liquid state and the solid glassy state. Good agreement is found in the $T_g(P)$ curve using the two methods. While the second method does not allow for quantitative determinations of the volume expansion coefficients of these systems, qualitative results can be obtained. It is found, e.g., that differences in the volume expansion coefficient upon crossing the glass transition are much greater for low-pressure fluids than for the much denser fluids at high pressure. Data will be presented for glycerol, an intermediate strength glass-forming system, as well as for the fragile glass former salol.

1This work was supported by NSF grants: DMR-0244180 and DMR-0552944.

2:42PM L27.00002 Pressure Raman experiments on Ge$_x$As$_{3-x}$Se$_1$-$_2$$_x$ glasses*, PING CHEN, P. BOOLCHAND, Univ. of Cincinnati — It is known that variations in the non-reversing enthalpy associated with glass transitions, $\Delta H_{nr}(x)$, display a global minimum (~0) in the 0.09 < $x$ < 0.16 range and the term increases at $x$ > 0.16 and at $x$ < 0.09 in the titled glasses. In this reversibility window, glasses are thought to in the Intermediate phase and form stress-free networks. Since the size of As, Ge and Se are nearly the same, Raman pressure experiments using a DAC provide a useful way to check the stress-free nature of glasses in the window. Preliminary results at $x$ = 0.11, and 0.14, compositions in the reversibility window, reveal Raman frequency of the symmetric stretch of Ge$_4$S$_4$ tetrahedra to blue-shift linearly with external pressure (P) once P>0. At $x$ = 0.18, a composition in the stressed-rigid phase, a blue-shift of the mode is also observed but only once P exceeds a threshold (P$_c$) value of 14 kbar. The present finding of a finite value of P$_c$, at $x$ = 0.18, but its vanishing at $x$ = 0.11 and 0.14, is quite similar to a previous one in binary Ge$_x$Se$_{1-x}$ glasses. We are now examining other glass compositions in the present ternary. * Supported by NSF grant DMR 04-56472 1 T. Qu et al. Mater. Res. Soc. Symp. Proc. 754, 111 (2003).


2:54PM L27.00003 Two Simple Models of Monoatomic Glass Formers, VITALIJ KAPKO, DMITRY MATYUSHOV, AUSTEN ANGELL, Arizona State University — Glass formation in one component systems remains a challenge for computer simulations, and therefore most studies to date have been done on binary mixtures. Here we explore the origin of resistance to crystallization of single component systems for two examples: modified silicon potential (Stillinger-Weber model) and Lenard-Jones ellipsoids (Gay-Berne model of liquid crystals). To produce glass formers these potentials were tuned by optimization of the parameter of three-body interaction (for the former) and aspect ratio (for the later). The kinetic properties and the potential energy landscapes of both models are studied.

3:06PM L27.00004 Tunable structures and properties in vitreous silica, LIPING HUANG, North Carolina State University, JOHN KIEFFER, University of Michigan — We studied the structures and properties of vitreous silica samples prepared by specific high pressure processing routes, using molecular dynamics simulations based on a charge-transfer three-body potential. Our study shows that the ability of the glass to undergo irreversible densification is inherently connected to its anomalous thermo-mechanical properties, such as the minimum in the bulk modulus at ~2-3 GPa and the negative thermal expansion while under pressure. These behaviors can be tuned by controlling the pressure under which the initial glass was quenched. By preparing silica glass in ways that eliminates anomalous thermo-mechanical behaviors, e.g., by quenching a melt under pressure, the propensity of the glass to undergo irreversible densification can be eradicated. Such “pressure-treated” silica glass is less susceptible to radiation damage and can potentially increase the lifetime of many optical components.

1NSF-DMR 0230662

3:18PM L27.00005 Molecular origin of the giant conductivity enhancement in (Ag$_2$S)$_x$(As$_2$S$_3$)$_{1-x}$ glasses, CHAD HOLBROOK, P. BOOLCHAND, University of Cincinnati — The solid electrolyte additive Ag$_2$S is found to homogeneously alloy with base As$_2$S$_3$ glass at low concentrations (x < 0.06, single: $T_g = T_g^{high} \sim 210$C), but it rapidly segregates as a Ag-rich glass phase at medium concentrations (0.06 < x < 0.20, bimodal: $T_g^{high}$ and $T_g^{low} \sim 170$C), and becomes the principal glass phase populated at higher x > 35 % (single: $T_g^{high}$) as revealed by modulated calorimetric measurements. The stoichiometry of the Ag-rich ($T_g^{low}$ phase) is suggested to be near AgAsS$_7$ at x < 25% but becomes closer to that of Smithite (AgAsS$_2$) at x > 40%, as revealed by Raman scattering. In the 9% < x < 14% composition range, one observes, in calorimetric experiments, the opening of a reversibility window, and a pronounced increase in the fractional population, R(x) of the Ag-rich glass phase, both of which correlate well with the 5-orders of magnitude increase in electrical conductivity across this compositional interval. In the same interval molar volumes on our samples show a local plateau. These observations suggest a new interpretation of the giant electrical conductivity enhancement observed at x > 15% in the present electrolyte glass system. 1 E.A. Kazakova and Z.U.Borisova, Fiz. Khim.Stekla 6, 424(1980).

1 NSF grant DMR 04-56472

3:30PM L27.00006 Enhanced Icosahedral Order in Supercooled Liquid Iron, P. GANESH, MIKE WIDOM, Carnegie Mellon University — As part of a study of metallic glass-forming ability, we perform first-principles molecular dynamics simulations of supercooled liquid iron. Analyzing the results according to the icosahedral order parameter $W_6$, we find that Iron exhibits enhanced icosahedral order compared with supercooled Copper and compared with dense random packing. Voronoi analysis confirms the enhanced order is in the form of 13-atom icosahedral clusters as well as characteristic Frank-Kasper type disclinated icosahedra. Upon further cooling the sample crystallizes to a BCC lattice, with the icosahedral clustering to form a novel point defect.

3:42PM L27.00007 Full Recovery of Electron Damage in Glass at Ambient Temperatures, ANDRE MKHOYAN, Cornell University, ADAM ELLISON, Corning, Inc., DIETER AST, RUEDIGER DIECKMANN, JOHN SILCOX, Cornell University — An unusually complete recovery of the electron beam induced damage in a CaO-Al$_2$O$_3$-SiO$_2$ glass was discovered. Nanoscale measurements carried out in a scanning transmission electron microscope show that the Ca ions migrate about 10 nm away during irradiation and return during recovery. Oxygen atoms are trapped largely as molecular oxygen and do not migrate. Electron energy loss measurements demonstrate that for glass to return completely to the original compositional and structural state the following processes must take place: First, no mass loss should occur. Thus the irradiation time should be less than the time necessary for significant mass-loss to occur. Second, diffusion must be sufficient at the ambient temperature for atoms to migrate back to suitable bonding sites. Third, the role of oxygen is critical: unless oxygen is available for recombination with the displaced atoms then recovery is incomplete. Finally, the observation that the system recovers so completely (structurally, as well as compositionally) after such a substantial perturbation is evidence that the initial state of the glass must be a very stable thermodynamic minimum [1]. 1 K.A. Mkhoyan et al., Phys. Rev. Lett. 96, 205506 (2006).

This work was supported by NSF EEC-0117770 and NYSTAR C020071.
3:54 PM L27.00008 Glass Transition and Structure in the Phase Field Crystal Model. Joel Berry, Martin Grant, McGill University, Ken Elder, Oakland University — The dynamics of the glass transition and structure of the disordered phase are studied using the Phase Field Crystal (PFC) model in two and three dimensions. It is shown that a kinetically driven glass transition is produced in 3D for sufficiently large cooling rates. Analysis of free energy barriers indicates that the glass phase is more accessible from the liquid than from the crystalline phase, but will not be stable for long times unless a critical cooling rate is exceeded. Below the critical cooling rate an equilibrium BCC structure is established. A Vogel-Fulcher type divergence in the density autocorrelation function is produced as the glass transition temperature is approached, signifying fragile glass forming behavior. As well the structure factor of the glass phase shows the characteristic split second peak. Notable differences between results in 2D and 3D will be discussed, as well as results for pure and binary systems.

4:06 PM L27.00009 Ion-conduction and rigidity/ flexibility of glasses1, D.I. Natives, P. Boolchand, University of Cincinnati, M. Malki, University of Orleans, M. Micoulaud, University of Paris — The (AgI)x(AlPO4)1−x solid electrolyte glass system has been examined extensively although a consensus on the increase of electrical conductivity with x data has been elusive. Here we show that the variability of the data is likely due to water contamination. Our work is on specifically prepared samples which display glass transition temperatures Tg(x) that are at least 50 °C to 100 °C higher than those reported hitherto. In Raman scattering the frequency of the P-O bonds in PO4 tetrahedra of long chains is found to systematically red-shift with increasing x, and to display thresholds near x = x(1) = 0.095(3)(stress-transition) and x = x(2) = 0.379(5)(rigidity transition). Calorimetric measurements show a reversibility window in the 0.09 < x < 0.38 range. Room temperature electrical conductivity, σ(x), increases with x to display thresholds near x(1) and x(2), and a logarithmic increase at x > x(2) with a power-law μ = 1.78(10) that is in good agreement with theoretical predictions2. Properties of flexibility and rigidity of backbones commonplace in covalent systems2 is a concept that extends to solid electrolyte glasses as well.

1Richard Zallen, Physics of Amorphous Solids
2P. Boolchand et al. Phil. Mag 85, 3823 (2005)

4:18 PM L27.00010 Locations of metal ions in the new glasses in the alumina-calcia-monazite (LaPO4) system1, Robert Marzke, George Wolf, Susan Bouchez, Jeremy Piwowarczyk, William Petuskey, Arizona State University — The new group of glasses synthesized from calcium aluminate (CaAl2O4) or Ca2Al7O12(CaO)xLa2O3(1-x) with varying fractions of La-monazite (LaPO4) has been characterized by electron microscopy, 31P and 27Al NMR, Raman scattering and chemical methods. These techniques have yielded information concerning the environments of the metal ions Al and La in the glasses. A substantial negative shift of the principal 31P NMR line at all monazite fractions, along with Raman spectra showing that PO4 groups do not share bridging oxygens, places La within the second coordination shell surrounding P. P-Al TRAPDOR double NMR experiments show that aluminum and phosphorus are also closely coordinated, accounting for a second, more negatively shifted line in the 31P single resonance spectra. Models for the structures of these glasses have been constructed for a range of monazite contents, and will be presented.

1Supported by NSF grant DMR 04-56472.

4:30 PM L27.00011 X-ray and Neutron Scattering Studies of Methyl Iodide Confined in GelTech© Glass, Yvonne Glanville1, Penn State University, Paul Sokol, Indiana University Cyclotron Facility, Steven Ehrlich, National Synchotron Light Source — X-ray diffraction and neutron scattering studies of methyl iodide confined in 200 Å GelTech© glass have revealed a never before observed intermediate solid phase of methyl iodide. Bulk methyl iodide has one phase transition below room temperature, at 207 K where it transitions from a liquid to an orthorhombic solid. Neutron scattering studies of the diffusion of methyl iodide confined in the 200 Å pores show a transition from a liquid to a solid at 203 K. X-ray diffraction measurements support this finding and identify the transition as one from a liquid to the never before observed amorphous solid. The amorphous solid remains down to 168 K upon cooling at which point a second transition appears from the amorphous solid to an orthorhombic solid, which upon indexing is identical to the bulk.

1Worthington Scranton Campus

4:42 PM L27.00012 Nonlinear susceptibility of the dipolar glass, Moshe Schechter, Philip Stamp, University of British Columbia — Glassy behavior is seen in various systems, among which are structural glasses, electron glasses, spin glasses and electric dipolar glasses. The latter two seem to share the same effective Hamiltonian. However, experimentally some fundamental differences are seen between these two systems, most notably the divergence of the nonlinear susceptibility in the spin glass system and its absence in the electric dipolar glass. Here we discuss the similarities and differences between these two systems leading to the above mentioned phenomenon.

4:54 PM L27.00013 Conductivity thresholds and glass structure in (K2O)(GeO2)1−x glasses1, Ninghua Wang, Deassy Novita, Punit Boolchand, University of Cincinnati — There are reports of conductivity thresholds with glass transition in solid electrolyte glasses. In the titled glass system, we show a order of magnitude increase in conductivity occurs at x > 0.10. The origin of the observation remains an open question. In titled glasses, we show that glass structure probe by the elastic behavior of its backbone shows two thresholds, a stress transition near x = 0.24 and a rigidity transition near x = 0.09. These elastic thresholds emerge from the reversibility window observed in calorimetric measurements, and in Raman scattering experiments that show scattering strength of the 520 cm−1 mode of 3-member rings to show a global maximum in the reversibility window. The pronounced increase of conductivity apparently occurs when backbones become flexible at x > 0.09, permitting K+ ions to freely diffuse. The correlation between the electrical, thermal and optical properties of the present solid electrolyte glasses may well be a generic feature of these materials.

1Supported by NSF grant DMR 04-56472.
2Jain et al. JNCS 222, 361 (1997).
3S. Chakravarty et al. J.C.M.P 17,L1-7 (2005).

Tuesday, March 6, 2007 2:30PM - 5:30PM —
Session L31 DCMP: Carbon Nanotubes: Superconductivity  Colorado Convention Center 401
2:30PM L31.00001 Carbon Nanotube Superconducting Quantum Interference Device. VINCENT BOUCHIAT, CNRS-Grenoble / Neel Institute, JEAN-PIERRE CLEUZIOU, CNRS-Toulouse /CEMES, THIERRY ONDARCUHU, MARC MONTIOUX, CNRS-Toulouse /CEMES, WOLFGANG WERNSDORFER, CNRS-Grenoble /Neel Institute — We report on the study of a superconducting quantum interference device (SQUID) with Josephson junctions made of portions of metallic single-walled carbon nanotube [1]. Quantum confinement in each nanotube junction induces a discrete quantum dot (QD) energy level structure, which can be controlled with a lateral electrostatic gate. In addition, a backgate electrode can vary the transparency of the QD barriers, thus permitting to change the hybridization of the QD states with the superconducting contacts [2]. The gates are also used to directly tune the quantum phase interference of the Cooper pairs circulating in the SQUID ring. Optimal modulation of a 6nA supercurrent with magnetic flux is achieved when both QD junctions are in the “on” or “off” state. Furthermore, the SQUID design establishes that these CNT Josephson junctions can be used as gate-controlled π-junctions. This allow to verify that the sign of the current-phase relation across a proximity coupled Qdot can be reversed with a gate voltage. Noise studies shows that the noise figure of the nanotube SQUID together with the size of the junction should allow the detection of a single molecule magnet. [1] J-P. Cleuziou et al. Nature Nanotec., 1, 53, (2006). [2] J-P. Cleuziou et al. cond-mat/0610622.

2:42PM L31.00007 Thermoelectric transport in the vicinity of a superconductor-metal quantum phase transition in nanowires. ADRIAN DEL MAESTRO, BERND ROSENOW, SUBIR SACHDEV, Harvard University — We consider a model of a zero temperature phase transition between superconducting and diffusive metallic states in very thin wires due to a Cooper pair breaking mechanism, e.g. a magnetic field in the wire direction or disorder in an unconventional superconductor. The critical theory contains current reducing fluctuations in the guise of both quantum and thermally activated phase slips. In a large-N limit, we calculate the universal dependence of the electrical and thermal conductivity on both pair breaking strength and temperature. We find that the conductivity has a non-monotonic temperature dependence on the metallic side of the transition and that the Wiedemann-Franz law is obeyed at low temperatures. In the quantum critical region, we study the dynamics of a two-component order parameter field via the Langevin equation formalism and compare with the large-N result.
3:54PM L31.00008 Superconductivity of nanowires in contact with bulk metals \(^1\), H. LIU, Z. YE, H. ZHANG, W. WU, Texas A&M University — A counter-intuitive anti-proximity effect (APE) was recently reported for Zn nanowires in contact with two superconducting bulk electrodes (PRL 95, 076802 (2005)). It was observed that the Zn nanowires were superconducting when the bulk electrodes were normal. When bulk electrodes were superconducting, superconductivity in the Zn nanowires appeared to be partially or fully suppressed. However, the resistance of the extrinsic contacts between the Zn nanowires and the bulk electrodes has raised questions about these experiments. To address this issue, we have fabricated Sn, Pb, and Zn nanowires of various diameters and lengths in contact with a number of different bulk materials using an in-situ contact method developed by our group (APL 84, 6996 (2004)) which eliminates any extrinsic contact resistance. Transport properties of the nanowires have been measured using a Physical Property Measurement System (PPMS). We have found that long (~60 μm) nanowires of Sn and Pb demonstrate superconductivity as expected with either superconducting or normal bulk electrodes. However, short (<10 μm) Sn and Pb nanowires demonstrate superconductivity only when the bulk electrodes are superconducting, such as Sn and Pb. Other samples with similar structures are being studied and will be used to clarify these results. We will discuss these results in the context of the proximity effect.

\(^1\)This work was supported by NSF under Grant No. DMR-0551813 and DMR-0606529.

4:06PM L31.00009 Magnetization drops in arrays of superconducting multi-walled carbon nanotubes, J. HARUYAMA, N. MURATA, Aoyama Gakuin University, E. EINARSSON, S. CHIASSI, S. MARUYAMA, Tokyo University, N. KISHI, T. SUGAI, H. SHINOHARA, Nagoya University — Superconductivity in CNT, which is an ideal one-dimensional (1D) conductor, is attracting significant attention, because it allows one to study how Cooper pairs can be generated and behave in 1D space within a ballistic charge transport regime. This study also reveals interplay between superconductive phase and phases of 1D quantum phenomena, which tend to prevent superconductivity from its appearance (e.g., Tomonaga-Luttinger liquid states and Piersl transition). We have recently reported finding of superconductivity with the highest Tc of 12 K for abrupt resistance drops in arrays of MWNTs by entirely end-bonding those by gold electrode [1]. Here, I will report finding of magnetization drops with the highest Tc of 18 K, which is greater than the above-mentioned Tc of 12 K, in the arrays of MWCTNs.Because only the samples with showing resistance drops can exhibit this magnetization drops, we conclude that this is attributed to Meissner effect. Based on this observation, we clarify that contribution of graphite structure of a MWNT is a dominant mechanism for the present Meissner effect rather than influence of curvature. We also reveal contribution of intertube coupling in an array of MWCTNs. [1] I.Takesue, J.Haruyama. et al., Phys.Rev.Lett. 96, 057001 (2006)

4:18PM L31.00100 Very Unusual Magnetic Properties in Multi-walled Carbon Mats, Pieder BEELI, GUO-MENG ZHAO, Department of Physics and Astronomy, CSULA — We report magnetic measurements up to 1100 K on a multi-walled carbon nanotube mat sample using a Quantum Design vibrating sample magnetometer. In an ultra-low field (\(H = -0.02\) Oe), we find a very large paramagnetic susceptibility (up to 12.77% of 1/4\(π\)) at 1100 K and a very large diamagnetic susceptibility (at least 8.4% of \(-1/4\)\(π\)) at 482 K. A small magnetic field (2.1 Oe) completely suppresses the diamagnetic susceptibility at 482 K and reduces the paramagnetic susceptibility at 1100 K by a factor of over 20. We rule out explanations based on magnetic contaminants, instrument artifacts, and the orbital diamagnetism. The magnetic data are inconsistent with any known physical phenomena except for granular superconductivity. The present results suggest the existence of an unknown new physical phenomenon or superconductivity with an ultra-high transition temperature.

4:30PM L31.00111 Lifetime of a one-dimensional fermion \(^1\), MAXIM KHODAS, William I. Fine Theoretical Physics Institute and School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA, IDDO USSISHKIN, Intel Corp., Israel, MICHAEL PUSTILNIK, School of Physics, Georgia Institute of Technology,Atlanta, GA 30332, ALEX KAMENEV, LEONID GLAZMAN, William I. Fine Theoretical Physics Institute and School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA — Interaction between fermions in one dimension is usually accounted for within the exactly soluble Tomonaga-Luttinger model. The crucial simplification made in this model is the linearization of the fermionic spectrum. That simplification leads to an infinite lifetime of a fermion at the mass shell, i.e., the corresponding Green function \(G(\xi, \xi)\) diverges at \(\varepsilon = \xi\). We find that inclusion of the curvature of electron spectrum, \(\frac{\xi_{\xi}}{\tau} = \frac{v_F k + k^2}{2m}\), yields a finite decay rate of a fermion, \(1/\tau(\xi) \propto \Theta(k) k^3/m^3\), here for definiteness we consider right-moving particles, and \(k\) is measured from the Fermi wave vector. The found finite lifetime allows one to assess the limitations of the Luttinger liquid paradigm.

\(^1\)NSF, Grants No. DMR02-37296, No. DMR-0405212, No. EIA02-10756, and A. P. Sloan Foundation.

4:42PM L31.00012 Electron Transport and Tunneling in Single Walled Carbon Nanotube Devices, TRAVIS DIRKS, NADYA MASON, Department of Physics, University of Illinois at Urbana-Champaign — Carbon nanotubes remain a fertile ground for the exploration of interacting one-dimensional (1D) physics and Tomonaga-Luttinger liquid theory. Much is still unknown about the factors that influence the transport and tunneling properties of interacting 1D systems such as nanotubes. We report on experiments that use techniques such as multiple contacts on long nanotubes and tunable tunnel barriers to determine how the manifestations of electron-electron interactions, such as the zero-bias anomaly, depend on the length and defect strength in nanotubes.


5:06PM L31.00014 The Study of Electron-Electron Interactions in Semi-Conducting Carbon Nanotubes Using a Numerical Renormalization Group, ROBERT KONIK, Brookhaven National Laboratory — We present a non-perturbative, numerical renormalization group (NRG) based technique for the study of the spectrum of semi-conducting single-walled carbon nanotubes in the presence of electron-electron interactions. This technique permits a full many-body treatment of the system. As our starting point, we model a single walled semi-conducting carbon nanotube as four gapped Dirac fermions in the presence of interactions. Focusing on a poorly screened carbon nanotube where the interactions are strongest in the forward scattering direction, the nanotube can be equivalently modeled as four Luttinger liquids coupled together with a quadratic gap term. The NRG based technique then is readily able to determine non-perturbatively the effects of the gap term upon the four Luttinger liquids. Using this approach we are able to obtain results for both the excitonic and single particle spectra of the nanotube.

THOMSON, JOHN WETTLAUFER, Yale University, LARRY WILEN, Ohio University — Near phase equilibrium, bulk properties of polycrystalline materials show a substantial increase in differential conductivity \((\Delta I/\Delta V)\) near zero voltage and a pronounced asymmetry with bias voltage that appear only below temperatures of 3.0K. The magnetic field peaks show complicated shifts and possible splits. The simplest interpretation that satisfies the data is that of a metallic tube whose Schottky barriers to the external contacts are asymmetric. The observation of a Kondo effect that varies with bias polarity dramatically illustrates the impact of coupling to the external leads.

Tuesday, March 6, 2007 2:30PM - 5:06PM — Session L41 DCMP: Ripples, Grain Boundaries, & Interfaces Colorado Convention Center 504

2:30PM L41.00001 Gas cluster ion irradiation in formation of nano-ripple structures on silicon surfaces and its applications to producing III-nitride nanorods, O. LOZANO, X.M. WANG, Q.Y. CHEN1, J.R. LIU, P.V. CHINTA, P.V. WADEKAR, WEI-KAN CHU, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, TX, H.W. SEO, Department of Physics, University of Arkansas, Little Rock, AR, L.W. TU, Y.T. LIN, Y.L. CHENG, Department of Physics and Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung, Taiwan, Republic of China — Gas cluster ion beams (GCIB) have been used to fabricate nano-ripple structures on Si substrates. In this work, using \((\text{Ar})^+_n\) clusters at 30 kV acceleration, where \(n=3,000\), we have observed nano-ripple formations on the silicon surface after GCIB bombardment. The wavelength, amplitude and the dimensions of the ripples were studied in an effort to characterize the morphology as a function of angle of incidence, crystallographic orientations of the substrate, and the ion dosages. The underlying physics of ripple formation will be discussed and fabrication of nanorods on rippled \((111)\)-Si substrates using III-nitrides, such as GaN, InGaN, and InAlN, will be presented.

1 also with Department of Physics and Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung, Taiwan, Republic of China.

2:42PM L41.00002 Studies of Ripple Formation on Si Surfaces During Ar\(^+\) Ion Bombardment, GOZDE OZAYDIN, Department of Aerospace and Mechanical Engineering, Boston University, Boston, MA, KARL F. LUDWIG, Department of Physics, Boston University, Boston, MA 02215, USA, HUA ZHOU, RANDALL L. HEADRICK, Department of Physics, University of Vermont, Burlington, VT 05405, USA — A study of formation of ripples on Si surfaces during bombardment with Ar\(^+\) ions is reported. Real-time grazing incidence small-angle x-ray scattering (GISAXS) measurements are performed at the National Synchrotron Light Source. Si \((100)\) samples are bombarded by Ar\(^+\) ions from a PHI sputter gun at off-normal incidence. The formation of ripple structures is monitored in real time. The effects of different ion energies and high temperatures on the formation of these ripples are studied. A separate study on the smoothing of ripples by ion bombardment at normal incidence is also performed. The real time smoothing of these ripples is monitored using GISAXS during ion bombardment of the surface at room temperature and at higher temperatures. The effects of ion energy and substrate temperature on the smoothing of ripples are discussed.

This work is partially supported by NSF DMR-0507351 and DOE DE-FG02-03ER46037.

2:54PM L41.00003 Vertical Asymmetry and the Ripple Rotation Transition in the Epitaxial Growth and Erosion on (110) Crystal Surfaces, LEONARDO GOLUMBOVIC, Physics Department, West Virginia University, ARTEM LEVANDOVSKY, Department of Chemical and Petroleum Engineering, University of Pittsburgh — We theoretically elucidate the ripple rotation transition on Ag\((110)\) crystal surface experimentally studied by de Mongeot and co-workers, as the transition between the Rectangular Rippled states (checkerboard structures of alternating rectangular pyramids and pits). We show that the experimental diffraction patterns can be understood only by invoking the vertical growth asymmetry. Interestingly, we find that the ripple rotation transition occurs over an extended parameter range: The transition point where the qualitative change of the near in-phase patterns occurs turns out to be different from the one where the change of the out-of-phase patterns occurs. In the proximity of the former transition point we find the four-lobe near in-phase diffraction pattern with the four peaks along the principal axed of the \((110)\) surface, in accord with the experiments on Ag\((110)\). Moreover, on the two sides of the extended ripple rotation transition, we find two novel interfacial states induced by the vertical asymmetry.

3:06PM L41.00004 Light scattering as a technique to probe grain boundary melting, ERIK THOMSON, JOHN WETTLAUFER, Yale University, LARRY WILEN, Ohio University — Near phase equilibrium, bulk properties of polycrystalline materials are strongly influenced by an interlinked network of grain interfaces. While numerical simulations and theory have supported the idea of disorder along grain boundaries, direct experimental access to the interface between two crystals of any material, in thermodynamic equilibrium, has been limited. The transparency, birefringency, and melting temperature of polycrystalline ice lend it to experimental probing. By scattering the collimated light of a 2.3 mW He-Ne laser off of the boundary of a hexagonal ice bi-crystal, prepared within a controlled ice growth cell, the boundary is directly explored. Reflected light intensity is measured as a function of the thermodynamic variables: temperature and impurity concentration. C-axis orientation can be determined by a systematic analysis of extinction angles for individual crystals held between cross polarizors. Assuming the index of refraction for bulk water, for any melted layer, a change in reflected signal is a function of the thermodynamic variables: temperature and impurity concentration. C-axis orientation can be determined by a systematic analysis of extinction angles for individual crystals held between cross polarizors.

3:18PM L41.00005 Adatoms, Grain Boundaries, and Thin Film Growth Stress, EDMUND WEBB III, Sandia National Laboratories, STEPHEN FOILES, CHUN-WEI PAO, DAVID SROLOVITZ, JERROLD FLORO — Atomicistic simulations will be presented revealing fundamental stress generation mechanisms during later stages of thin film growth when substrate coverage is complete and the film is thickening. Typically, films exhibit texture with grain boundaries intersecting the surface. In situ growth stress experiments reveal compressive stress generation during this stage; if growth is interrupted, experiments show a relaxation in compressive stress with a characteristic rate. An existing theory proposes that, during deposition, adatoms incorporate into grain boundaries, generating compressive stress. However, debate exists regarding this mechanism and data observed in growth interrupt experiments. Simulations will demonstrate that adatoms are strongly attracted to grain boundaries and readily incorporate into them. Furthermore, adatom incorporation generates compressive stress in accord with experiments. A model is presented establishing a quantitative link between adatom incorporation into grain boundaries and the resultant stress generated.
3:30PM L41.00006 Grain-boundary grooving and agglomeration of alloy thin films: phase-field simulations

MATHIEU BOUVILLE, DONGZHI CHI, Institute of Materials Research and Engineering, DAVID J. SROLOVITZ, Yeshiva University — A common failure mode in polycrystalline thin films is grain-boundary grooving through the thickness of the film. This can bring the surface in contact with the substrate, leading to film agglomeration. Although grain-boundary grooving has received a great deal of attention over the past half-century, the extant models are too idealized to be useful to predict agglomeration in most technologically interesting materials, such as multicomponent alloy films. We relax many of the assumptions made in the classical analysis, thereby finding unprecedented richness in the problem. Our approach employs a phase-field model for grain-boundary grooving and agglomeration of polycrystalline alloy thin films. In particular, we study the effects of slow-diffusing species on grooving rate. As the groove grows, the slow species becomes concentrated near the groove tip so that further grooving is limited by the rate at which it diffuses away from the tip. At early times the dominant diffusion path is along the boundary, while at late times it is parallel to the substrate. This change in path strongly affects the time-dependence of grain-boundary grooving and increases the time to agglomeration. The present model provides a tool for agglomeration-resistant thin film alloy design.

1 DOE (DE-Fg-03ER45575)

3:42PM L41.00007 Enhanced growth instability of strained film on curved substrate

YU ZHANG, HANGYAO WANG, FENG LIU — We report linear stability analysis of a strained film on a curved surface. We show that the growth of a strained film is inherently less stable on a curved substrate than on a flat substrate. For small surface undulation, the lowest strain energy state is for the film surface to adopt the same wavelength as the substrate surface in an anti-phase configuration. Our analysis provides some qualitative understanding of directional self-assembly of quantum dots on patterned substrates.

3:54PM L41.00008 Si-Ge Intermixing and the 5x5-(111) Surface Reconstruction

DEMETRA PISACHOS, M. J. STOTT, Department of Physics, Queen’s University — We present ab initio results of the energetics and structure of a Si(111)-5x5 slab with two bilayers of Ge(5x5) adsorbed on it. We explore the aspects of this Si-Ge surface structure with those of an analogous pure Ge(111)-5x5 slab and we note many important differences such as the larger corrugation of the adatom heights in the former compared with the latter. Ab initio results are also obtained for the effects of Si-Ge intermixing at the Si-Ge interface. These shed light on this transport mechanism as a way of lowering the strain.

1 Work supported by the NSERC of Canada

4:06PM L41.00009 Ti as an Interface Stabilizer for Fe/Al and Al/Fe Interfaces

W. PRIYANTHA, A. COMOUTH, A. KAYANI, H. CHEN, M. KOPCZYK, R.J. SMITH, Montana State University, Bozeman, MT, D. MCCREADY, Pacific Northwest National Laboratory, Richland, WA — The use of ultra-thin metal interlayers to stabilize metal-metal interfaces and to limit interdiffusion has drawn much attention over the past few years, driven by a variety of technological applications. Earlier we reported that using a Ti monolayer as an interlayer stopped diffusion at the Fe/Al(001) interface. These findings encouraged us to explore the use of interlayer structures for thin films of technological interest deposited on Si wafers at room temperature using RF sputtering. AlFe and FeAl metal layers, with and without a Ti stabilizing interlayer, were studied using Rutherford backscattering (RBS) and X-ray reflectivity (XRR). Analysis revealed that FeAl and AlFe films without a Ti interlayer on SiO2/Si wafers showed considerable Fe-Al intermixing, especially when the Fe layer was deposited on top of the Al layer. With a Ti interlayer present at the interface both AlFe and FeAl interfaces exhibited less interdiffusion.

1 This work was supported by the National Science Foundation, NSF Grant DMR 0516603.

4:18PM L41.00010 Impurity Segregation at the Si/SiO2 Interface

A. G. MARINOPoulos, K. VAN BENTHEM, S. RASHKEEV, S. J. PENNYCOOK, S. T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235 and Oak Ridge National Laboratory, Oak Ridge, TN 37831 — It is a widely known fact that impurities tend to segregate at interfaces between two materials. Here we report results of the energetics and structure of a Si(111)-5x5 slab with two bilayers of Ge(5x5) adsorbed on it. These findings encouraged us to explore the use of interlayer structures for thin films of technological interest deposited on Si wafers at room temperature using RF sputtering. AlFe and FeAl metal layers, with and without a Ti stabilizing interlayer, were studied using Rutherford backscattering (RBS) and X-ray reflectivity (XRR). Analysis revealed that FeAl and AlFe films without a Ti interlayer on SiO2/Si wafers showed considerable Fe-Al intermixing, especially when the Fe layer was deposited on top of the Al layer. With a Ti interlayer present at the interface both AlFe and FeAl interfaces exhibited less interdiffusion.

4:30PM L41.00011 Temperature Induced Modifications of SiC Interfaces studied by High Resolution Electron Energy Loss Spectroscopy

J.A. SCHAEFER, M. EREMTCHENKO, J. UHLIG, A. NEUMANN, R. OETTKING, S.I.-U. AHMED, Institut fuer Physik und Institut fuer Mikro- und Nanotechnologien, Technische Universitaet Ilmenau — High resolution electron energy loss spectroscopy (HREELS) is a fascinating tool for studying electronic and vibrational properties in the near surface regime. For SiC, a wide band gap semiconductor suited for several applications, the surface and interface chemical reactivity needs to be thoroughly understood. In addition to atmospheric adsorbates, C- and Si-terminated cub- and hex-SiC, changes in carrier concentration profiles and band bendings can be monitored by comparing HREELS-data with dielectric theory. There, the surface state density related to the reconstruction type and surface composition is important together with the substrate temperature. For oxygen on 6H-SiC (0001), we observed for the first time new vibrational modes linked to distinct Si-O-Si vibrations, namely its asymmetric- and symmetric stretching vibrations and wagging motion. The energy and intensity of the asymmetric stretching frequency is analogous to the initial stage oxidation of Si surfaces.

1 Financial support was provided by the Deutsche Forschungsgemeinschaft (DFG) under grant Sch4 435/17-1.

4:42PM L41.00012 ABSTRACT HAS BEEN MOVED TO X19.00015
4:54PM L41.00013 Measurement of Young’s modulus of thin films using modal characterization. 3  
DRAGOSLAV GRBOVIC, NICKOLAY LAVRIK, PANOS DATSKOS, University of Tennessee, Knoxville, TN 37996 and Oak Ridge National Laboratory, Oak Ridge, TN 37931 — We present a method for experimentally measuring Young’s modulus of thin films using micro-electro-mechanical systems (MEMS). Properties of thin films often differ from those in bulk material and, moreover, depend on deposition method. In this work, we describe the results of measurements of Young’s modulus of titanium (Ti) thin film deposited by sputtering. We deposit Ti on microcantilever structures with specified dimensions and known material properties and then experimentally measure the frequency shifts for the first several resonant modes. Using the acquired resonant frequencies in finite element analysis, we obtain the Young’s modulus of the deposited Ti film. Our results show that Young’s modulus of Ti film deposited by sputtering varies with thickness from ~60 GPa for 35 nm film to ~73 GPa for 100 nm film. This approach is fast and independent of material or deposition method. It is especially valuable in determining effective Young’s moduli of composite and nanostructured thin film materials with complex relationships between their composition and their properties.

Tuesday, March 6, 2007 2:30PM - 5:18PM — Session L42 DCMP: Excitations at Surfaces Colorado Convention Center 505

2:30PM L42.00001 Low-Energy Acoustic Collective Excitations on Metal Surfaces  
BOGDAN DIACONESCU, KARSTEN POHL, University of New Hampshire, US, LUCA VATTUONE, LETIZIA SAVIO, Università di Genova, Italy, PHILIP HOFMANN, University of Arizona, Denmark, VYACHESLAV SILKIN, Facultad de Ciencias Quimicas, Spain, JOSE PITARKE, Zientzi Fakultatea, Spain, EUGENIE CHULKOV, PEDRO ECHENIQUE, Facultad de Ciencias Quimicas, Spain, DANIEL FARIAS, Universidad Autonomia de Madrid, Spain, MARIO ROCCA, Universita di Genova, Italy — Sound-like longitudinal plasma waves where thought to only exist in layered systems where spatially separated 2D electron plasmas are realized. Due to their low energy and linear dispersion such waves were proposed as possible candidates to mediate the attractive interaction leading to the formation of Cooper pairs in high TC superconductors. A new type of collective excitation mode on metal surfaces has been found. In contrast to the usual surface plasmon, it has an acoustic dispersion. For Be(0001) the mode was observed using EELS. Detailed ab-initio calculations show that it is caused by the coexistence of a partially occupied quasi-2D surface state band with the underlying 3D continuum in the same region of space. While it exists up to high energies for Be(0001), the mode as such has a very general character, for low energies it is expected to exist on many surfaces, profoundly affecting their electron and phonon dynamics.  

2:42PM L42.00002 Raman and infrared study of synthetic Maya pigments as a function of heating time and dye concentration  
LAYRA REZA, FELICIA MANCIU, LORI POLETTE, BRENDA TORRES, RUSSELL CHIANELLI, UTEP — Maya Blue is a famous indigo-based pigment produced by the ancient Mayas. Samples for the present work are made by a synthetic route, and demonstrate similar chemical stability as the ancient Maya Blue samples. Since no direct proof exists that the indigo chemically binds to the inorganic palagorskite lattice, there are still controversies on the resting place of the indigo molecules; i.e. are they in the channels of palagorskite, on the surface, or both. Our analysis, by FT-Raman and FT-IR spectroscopy proves the partial elimination of the selection rules for the centrosymmetric indigo, and shows the disappearance of the indigo N-H bonding, as the organic molecules incorporate into palagorskite material. Infrared data confirm the loss of zeolitic water and a partial removal of structural water after the heating process. Evidence of bonding between cationic aluminum and indigo through nitrogen is revealed by FT-Raman measurements. The oxygen carbonyl is also believed to interact with the metal.

2:54PM L42.00003 Infrared Spectroscopy of the Elastically-Strained Silicon Nanomembrane Bonding Interface  
ARNOLD KIEFER, WEINA PENG, DONALD SAVAGE, MAX LAGALLY, University of Wisconsin Madison — We investigate the bonding interface between elastically strained silicon nanomembranes (SiNMs) and new host substrates with Fourier transform infrared spectroscopy in efforts to elucidate its chemical structure. We create SiNMs by heteroepitaxial growth of strainning layers on the template layer of silicon-on-insulator (SOI) and then releasing the membrane sandwich by etching away the buried oxide. We then bond the SiNM to a new substrate, in the present case oxidized Si. Because the SiNM is only nanometers thick, the bonding interface contributes greatly to the membrane’s structural and electrical properties. We probe the buried interface by attenuated total reflection via the evanescent wave from a germanium prism in intimate contact with the SiNM, which penetrates through the SiNM to interact with the interface bonds. In efforts to understand bond strength and interface electronic states, we probe the influence of different cleaning procedures, gas treatments, and annealing steps.

3:06PM L42.00004 Dynamical Properties of Surface-mounted Dipolar Molecular Rotators  
JASON UNDERWOOD, JOHN PRICE, University of Colorado, Department of Physics, DOUGLAS CASKEY, JOSEF MICHL, University of Colorado, Department of Chemistry and Biochemistry — We use dielectric relaxation spectroscopy (DRS) to study the rotational dynamics of dipolar molecules mounted on fused SiO2 surfaces. Each “molecular rotor” consists of three parts: 1) a mounting group for attachment to the substrate, 2) a rotating group having a permanent dipole moment, and 3) an axis connecting the rotor to the attachment group. Attachment is facilitated either by covalent bonding through reaction of silane groups with surface hydroxyl or by van der Waals interactions. Fused SiO2 substrates are patterned with interdigitated electrode Au capacitors (C ≈ 1 pF), and rotor molecule dynamics are characterized by measurement of the capacitance C and loss tangent tan δ ≅ Re[Z]/Im[Z]. We employ a ratio-transformer bridge technique to measure these quantities, with sensitivities in C and tan δ of 1 aF and 1 ppm, respectively. A unique aspect of this work is the experimental apparatus, which allows us to prepare sub-monolayer films, determine coverage via two independent methods (DRS and XPS), and study molecule rotational motion, in-situ in ultra-high vacuum. Results will be presented on the kinetics of rotor adsorption/desorption, barrier height and asymmetry of the rotational potential of the molecules, and the effects of varying rotor coverages and adventitious H2O.

3:18PM L42.00005 Optical and opto-electronic based velocity and topographic measurements of a laser-ablated thin-metal layer on glass  
ANTHONY VALENZUELA, GEORGE RODRIGUEZ, Materials Physics and Applications Div., Los Alamos National Laboratory, STEVEN CLARKE, KEITH THOMAS, Weapons System Engineering Div., Los Alamos National Laboratory — We report on our ability to resolve the velocity and spatial profile of ablatively launched metal with nano-scale precision. We utilize a nanosecond laser pulse to launch a thin layer of titanium metal from a glass surface. Subsequently, we use optical and opto-electronic devices to diagnose the velocity and topography of the launched thin layers. Doppler Emission Velocimeter (PDV) utilizes the heterodyne principle that allows us to track multiple velocity components. Our topographer incorporates a Shack-Hartmann interferometer to provide details of the deformation of the surface as it is launched. We compare the experimental data to simulations to provide a feedback loop to improve our theoretical models. We also discuss possibilities to extend the sensitivity of the PDV system to provide a compact diagnostic with a broad range of capabilities.
3:30PM L42.00006 Surface Plasmon Assisted Kondo Resonances on a Metallic Nanowire, REN-SHOU HUANG, YIA-CHUNG CHANG, Research Center for Applied Sciences, Academia Sinica — We propose an experiment to measure the Kondo effect for magnetic atoms adsorbed on the surface of a metallic nanowire. In addition to the traditional \( sp-d \) hybridization, by introducing the strong electromagnetic field of the localized surface plasmon on the nanowire, we show that it is possible to observe additional \( sp-d \) electron transfer processes assisted by surface plasmons. Due to the good surface-to-volume ratio of the nanowire, the Kondo resonances could be observed as multiple anti-resonances in the differential conductance versus bias voltage curve.

3:42PM L42.00007 Positronium physisorption at quartz surfaces\(^1\), ROLANDO SANIZ, ARTHUR FREEMAN, Northwestern University, BERNARDO BARBIELLI, Northeastern University, PHIL PLATZMAN, Bell Laboratories — The possibility of having positronium (Ps) physisorbed at a material surface is of great fundamental interest, since it can lead to new insight regarding quantum sticking and is a necessary first step to try to obtain a Ps\(_2\) molecule on a material host. Experimental evidence for physisorbed Ps at the surface of quartz was reported some years ago but firm theoretical support for such a conclusion was lacking. With the FLAPW method\(^2\) we calculated the electronic structure and dielectric function of \( \alpha \)-quartz and obtained the interaction potential with a Ps atom on its surface. We show that there is indeed a bound state with an energy of \( \sim 0.19 \) eV, which is reasonably close to the experimental estimates of 0.14 - 0.17 eV. A brief energy analysis in terms of the Langmuir-Hinshelwood mechanism further shows that the formation of a Ps\(_2\) molecule at quartz surface would be possible.

3:54PM L42.00008 Molecule-resolved structural and electronic properties of diamondoid self-assembled monolayers\(^1\), JASON C. RANDEL\(^2\), HARI C. MANOHARAN\(^3\), Stanford University — Diamondoids represent an exciting new direction in the field of nanoscale carbon. While structurally and electronically stable, diamondoids have been experimentally inaccessible due to synthesis roadblocks and lack of natural sources, until recently purified from crude oil. We investigate the local structural and electronic properties of self-assembled monolayers formed from thiol-functionalized diamondoids. Using a high-throughput vacuum scanning tunneling microscope, we observe these monolayers to be robust and stable up to room temperature. Topographic data demonstrate well-ordered lattices for all molecules studied (adamantane through tetramantane), with lattice constants and angles that vary with polycrystalline order. Tuning spectroscopy reveals a conductance gap in the energy spectra of each molecule, which we compare to calculated HOMO-LUMO gaps and band alignments. The hierarchical nature of these molecules, and the ability to functionalize them with specific atomic and molecular end groups, provide a new set of customizable molecular nanomaterials.

4:06PM L42.00009 X-Ray Photoemission Analysis of Chemically Treated CdZnTe Semiconductor Surfaces, ART NELSON, LLNL, DANIEL VAZQUEZ, UC Santa Barbara, ANN BLISS, CHERYL EVANS, JIM FERREIRA, REBECCA NIKOLOC, STEVE PAYNE, LLNL — Device-grade Cd\(_1-x\)Zn\(_x\)Te was subjected to various chemical treatments commonly used in device fabrication to determine the resulting microscopic surface composition/morphology and the effect on contact formation. Br-MeOH (2\% Br), \( \text{N}_2\text{H}_4\text{F}/\text{H}_2\text{O}_2 \), and \( \text{(NH}_4\text{)}_2\text{S} \) solutions were used to modify the surface chemistry of the Cd\(_1-x\)Zn\(_x\)Te crystals. Scanning electron microscopy was used to evaluate the resultant surface morphology. Angle-resolved high-resolution photoemission measurements on the valence band electronic structure and Zn 2p, Cd 3d, Te 3d, O 1s core lines were used to examine the chemistry of the chemically treated surfaces. Metal overlayers were then deposited on these chemically treated surfaces and the I-V characteristics were measured. The measurements were correlated to understand the effect of interface chemistry on the electronic structure at these interfaces with the goal of optimizing the metal/Cd\(_1-x\)Zn\(_x\)Te Schottky barrier for radiation detector devices. This work was performed under the auspices of the U.S. Dept. of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

4:18PM L42.00010 On the role of multiple hot electron processes in STM-induced atom motion on surfaces, J. W. GADZUK, NIST — The phenomenon of adsorbed atom excitation/manipulation induced by hot-electrons delivered to the surface by an STM tip is related to desorption induced by multiple electron transition (DIMET) processes in which femtosecond laser pulses excite substrate electrons, creating a flux of hot electrons incident upon the surface from within rather than externally as occurs with the STM. While the sources of the hot electrons differ, the individual inelastic electron scattering processes giving rise to atomic motion over activation barriers are identical. This facilitates an adaptation of DIMET theory\(^1\) to multiple-electron STM surface processing. Recent relevant experiments: i) STM-induced non-local hot electron dissociation of dimethylsulfide on Au (111) by Maksymovych and Yates; ii) “below-one-electron-threshold” excited motion of single Co atoms on Cu (111) by Stroscio and coworkers will be considered in the light of a DIMET-based theory that focuses on special aspects of multiple excitation processes. [1] J. W. Gadzuk, Chem. Phys. Vol.251, 87 (2000).

4:30PM L42.00011 Probing the mechanism of infrared resonant desorption of hydrogen from Si(111): anharmonicity and energy pooling\(^1\), ZHIHENG LIU, LEONARD FELDMAN, NORMAN TOLK, Vanderbilt University, ZHENYU ZHANG, Oak Ridge National Laboratory, PHILIP COHEN, University of Minnesota — Desorption of hydrogen from a Si(111) surface by resonant infrared excitation of the Si–H vibrational stretch mode requires vibrational ladder climbing of a Si–H bond to a high level leading to associative desorption. We report recent experiments probing the mechanism of ladder climbing. H\(_2\) desorption is observed when the excitation linewidths are narrower than the anharmonicity of the Si–H bond, favoring energy pooling over multiphoton absorption. The resonance width of H\(_2\) desorption with an excitation linewidth of 8.7 cm\(^{-1}\) is measured to be 39 cm\(^{-1}\), opening a new opportunity for site-selective modification on the Si(111) surface. The desorption yield decreases when the sample temperature increases, consistent with an energy pooling process.

\(^1\)This work is funded by DARPA/SPAWAR grant N00014-04-1-8924, DOE grant ER45781, and NSF grant DMR-0306239.
4:42PM L42.00012 Probing Electron-Hole Pair Production in Ultrathin Film Schottky Diode Devices using Hyperthermal Energy Ion Beams.\(^1\) MATTHEW RAY, RUSSELL LAKE, CHAD SOSOLIK, Clemson University, CLEMSON UNIVERSITY DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING COLLABORATION — We are investigating the interactions of hyperthermal energy ions with ultrathin film Schottky diode devices, probing the role of ion-surface impact events and charge transfer on electron-hole pair production. Specifically, we measure currents that arise from electron-hole pair production at a diode surface. To date, these currents have been explored only for thermal energy gas-surface impacts, where they are called "chemicurrents". Using a UHV beamline to produce well-collimated monoenergetic noble gas and alkali-metal beams from 10 eV to 10 keV, we have the unique flexibility to probe our in-house designed diode devices with a wide range of incident species, energies, and charge states. Preliminary results are presented and discussed in the context of basic gas-surface energy transfer processes.

\(^1\) NSF-CHE CAREER

4:54PM L42.00013 Characterization of the Unoccupied Electronic Structure of Alkali Atoms on Noble Metal Surfaces by Time- and Angle-Resolved Two-Photon Photoemission. VAHIT SAME-TOGLU, University of Pittsburgh, AINO WINKELMANN, Max-Planck-Institut, JIN ZHAO, HRVOJE PETEK, University of Pittsburgh, NIKO PONTIUS, BESSY mbH, ANDREI BORISOV, Université Paris-Sud, PEDRO ECHENIQUE, Universidad del Pas Vasco, UNIVERSITY OF PITTSBURGH TEAM, MAX-PLANCK-INSTITUTE COLLABORATION, BESSY MBH COLLABORATION, UNIVERSITÉ PARIS-SUD COLLABORATION, UNIVERSIDAD DEL PAIS VASCO COLLABORATION — We perform angle-resolved two-photon photoemission (2PPE) spectral measurements on alkali atom (Li - Cs) covered noble metal (Cu(111) and Ag(111)) surfaces. The progressive evolution of 2PPE spectra with the alkali atom coverage is measured in the 0 - 0.1 monolayer range. We report on the dependence of 2PPE spectra on the alkali atom coverage, the photoemission angle, and the excitation laser polarization. The spectral measurements provide new information on the nature of chemisorption of alkali atoms on noble metals, as well as the photoinduced charge transfer excitation of alkali atoms. A general model for the image charge interactions at metal surfaces reproduces the experimental electronic structure quantitatively.

5:06PM L42.00014 Phononic and nonlocality contributions to Second Harmonic Generation in NiO. WOLFGANG HUEBNER, GEORGIOS LEFKIDIS, Kaiserslautern University of Technology — The experimentally observed second harmonic signal in centrosymmetric NiO can be explained with symmetry lowering mechanisms: (i) signal from the surface, (ii) spin-orbit coupling, (iii) nonlocalities, and (iv) lattice distortions [1]. First the intragap energy levels of both the (001) surface and the bulk of NiO are obtained with highly correlated quantum chemistry methods: single excitation configuration-interaction, and multiconfigurational complete active space, optimizing each d-level separately. Then the second-order susceptibility tensor is calculated beyond the electric-dipole approximation. The effects of spin-orbit coupling are studied, and a detailed analysis of the effects of the inclusion of nonlocalities from magnetic dipoles and electric quadrupoles is performed. Finally the effects of phonons in the bulk of NiO within the frozen phonon approximation are included, and the second order susceptibility tensor is computed both in a time resolved and time averaged manner [2].


Tuesday, March 6, 2007 2:30PM - 5:30PM — Session L43 DCMP: Optical Properties of Quantum Dots and Nanowires

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2:30PM L43.00001 Magneto-Optical Studies of PbSe Colloidal Nanostructures. J.G. TISCHLER, T.A. KENNEDY, E.R. GLASER, E.E. FOOS, T.J. ZEGA, R.M. STROUD, A.L. EFROS, S.C. ERWIN, Naval Research Laboratory — PbSe is an unusual semiconductor material with a direct band gap at the L point of 150 meV at 4 K. The band structure at this symmetry point is four-fold degenerate for both electrons and light holes, and conduction and valence bands possess similar effective masses and g-factors. Since both masses are relatively small, quantum confinement effects are easily achieved by reducing the nanocrystal size to dimensions of the order of the large exciton Bohr radius, \( a_B \approx 46 \text{ nm} \). We synthesized high quality PbSe nanocrystals and characterized them using transmission electron microscopy and optical methods. We probed the g-factor and fine structure of excitons in undoped PbSe quantum dots using optically detected magnetic resonance (ODMR) at 24 GHz and polarized photoluminescence in a magnetic field. The ODMR reveals that the g-factor is large for electron and holes (\( g = 7.6 \)) compared to other semiconductor nanocrystal systems. The photoluminescence polarization increases linearly with increasing magnetic fields up to 6 T, indicating that the fine-structure splitting is rather small.

2:42PM L43.00002 Multiple exciton generation in films of chemically treated lead chalcogenide quantum dots. JOSEPH LUTHER, NREL, MATTHEW BEARD, JAMES MURPHY, RANDY ELLINGSON, MATT LAW, KELLY KNUTSEN, ARTHUR NOZIK — Multiple exciton generation (MEG) is a unique process, which allows nanocrystals to produce several electron-hole pairs if the excitation energy is high compared to the bandgap of the material. Although the exact process that occurs in MEG is still under debate, the existence of the phenomenon is proven for quantum dots (QDs) in solution. This unique process leads to a desire to fabricate photovoltaic devices, among other things, which would benefit from the enhancement in photocurrent produced at short wavelengths. The fabrication of devices is problematic because the QDs must be close enough for charge transport to occur, yet remain confined for the process of MEG. In our work, we discuss how the exciton dynamics including MEG are affected by assembling the QDs into neat ordered arrays using transient absorption spectroscopy. The inter-QD distance is varied by treating the as-prepared array in dilute solution of short-chained amines.

2:54PM L43.00003 Surface Termination Effects on Zinc Oxide Quantum Dots. JOE SPALENKA, CHRISTOPHER JACK, CARY ALLEN, REUBEN COLLINS, THOMAS FURTAK, Colorado School of Mines — We investigate the effects of surface terminations on the optical properties of 2-6 nm ZnO quantum dots. Nanocrystals were grown by wet chemical synthesis in a short-chain alcohol solvent from zinc acetate and sodium hydroxide. Quenching of particle growth with various capping agents is necessary to maintain and enhance the unique characteristics of the nanocrystals. We reproduce results of previous work and expand on characterization of naked and surface terminated ZnO quantum dots. The nanoparticle properties were investigated by UV absorption spectrophotometry, photoluminescence, infrared spectroscopy, scanning electron microscopy, and atomic force microscopy techniques.

This material is based on work supported by the National Science Foundation under Grant No. DMR-0606054.
while that of the dot with radius 1.36 nm is 0.295 eV for the spin three-half state and 0.261 eV for the spin one half-state. The system increases. We get that the trion binding energy of the dot with radius 1.09 nm is 0.242 eV and 0.227 eV for the spin three-half and one-half respectively. We confirm that the binding energy decreases as the size of the QD decreases, thus doping in small Si QDs becomes more difficult. We explain the general chemical trends and the variation as a function of size and shape, based on first principles, Density Functional Theory calculations. In particular, we discuss the relative influence of quantum confinement and surface effects, and propose a way to monitor dielectric properties changes at the nanoscale, based on the development of novel highly-efficient solar photoconversion approaches. The efficient generation of multiple excitons following absorption of a single photon in semiconductor nanocrystals (NCs) represents one possible route towards inexpensive, high-efficiency solar cells. The multiple exciton state, which has been observed for absorption of a single photon with energy above twice the NC effective bandgap in various colloidal semiconductors, can be detected through the Auger recombination signature in the decay of the charge carrier population. Exciton population decays can be measured by studying the time-dependence of either intra- or inter-band photoinduced absorption, or via the decay of photoluminescence for emissive samples. We report on work in our laboratory to study multiple exciton generation, and its potential for solar energy conversion applications, in various lead-salt as well as II-VI semiconductor nanocrystals. The general chemical trends found in the QDs are similar to those found in bulk Si. We show that defect formation energy and transition energy level increase when the size of the QDs decreases, thus doping in small Si QDs becomes more difficult. We explain the general chemical trends and the variation as a function of size and shape, based on first principles, Density Functional Theory calculations. In particular, we discuss the relative influence of quantum confinement and surface effects, and propose a way to monitor dielectric properties changes at the nanoscale, based on the development of local dielectric response functions. Understanding the doping properties in Si QDs are very important for both theory and experiment. Using first-principles methods, we have systematically calculated the defect formation energies and transition energy levels of group-III and group-V impurities doped in Si QDs as functions of the QD size. The general chemical trends found in the QDs are similar to those found in bulk Si. We show that defect formation energy and transition energy level increase when the size of the QD decreases, thus doping in small Si QDs becomes more difficult. We explain the general chemical trends and the variation as a function of size in terms of the atomic eigenvalues and quantum confinement effects. We also calculate the absorption spectrum of size-dependent Si QDs and quantum rods by large-scale “charge patching method”. We show that the band gap and optical transitions of Si nanocrystals can be tailored continuously by size or shape. These results provide guidelines for future device design that require the knowledge of the size/shape-dependence of the nanocrystal’s electronic and optical properties.
4:18PM L43.00010 Internal transitions of singlet and triplet charged excitons in quantum dots1, A. DZUBYENKO, California State University Bakersfield, A. SIWACHENKO, Anadine Genomics Inc. — We theoretically studied the spectra of internal transitions of spin-singlet and spin-triplet charged excitons $X^\pm$ in quantum dots in finite magnetic fields. The lateral confinement in quantum dots was modeled by a parabolic potential. Both equal and different oscillator lengths for electrons and holes were considered. The states of charged excitons were found using the expansion in Fock-Darwin in-plane states and in size-quantization levels in quantum wells of different widths. We performed systematic studies of the spectra dependencies on the quantum well width, on the regime of lateral confinement, and on the magnetic field strength. In the absence of lateral confinement, the spectra of internal transitions are governed by a non-selective optical selection rule that follows from the rotational symmetry and magnetic translations. The selection rule prohibits, in particular, a triplet bound-to-bound inter-Landau level transition with energies below the electron cyclotron resonance. When the magnetic translational symmetry is broken by the lateral confinement, the previously prohibited transitions become allowed and acquire finite oscillator strengths. We compare our theoretical results with the existing experimental data on internal excitonic transitions in interface fluctuation quantum dots in GaAs QWs.

1Supported in part by NSF grants DMR-0203560 and DMR-0224225, and by a College Award of Cottrell Research Corporation

4:30PM L43.00011 Optical Phonon Modes in GaAs Nanowires, E. SPEISER, W. RICHTER, CNISM, Fisica, Roma Tor Vergata, Via della Ricerca Scientifica 1, I-00133 Roma, Italy, P. PRETE, IMM del CNR, Unità di Lecce, Via Arnesano, I-73100 Lecce, Italy, P. PAIANO, N. LOVERGINIE, CNISM, Unità di Lecce and Dipartimento di Ingegneria dell’Innovazione, Universita di Lecce, Via Arnesano, I-73100 Lecce, Italy. — We report micro Raman scattering spectra from free-standing Au-catalyzed self-assembled GaAs nanowires on (111)B GaAs grown by metalorganic vapor phase epitaxy. The nanowires are [111]B aligned and kink-free. Their base diameter distribution is narrow (11.4 nm standard deviation) and closely matches the size (60 nm) of the Au nanoparticles at their tip. Depending on the exciting laser power density (several hundred $\mu$W/µm²) the Raman spectra of the nanowires show thermally induced frequency shifts and broadening of the Raman lines. Series of power dependent spectra allow to extrapolate the phonon line shape and frequency free from thermal effects. The two main Raman lines corresponding to TO and LO of the bulk do not show frequency shifts with respect to the bulk. However, the Raman spectra exhibit new vibrational modes appearing in the gap between the TO and LO phonon lines. The appearance of those lines is sensitive to the polarization of the laser light. Raman spectra from AlGaAs nanowires will also be discussed with respect to the AlGaAs stoichiometry.

4:42PM L43.00012 Influence of the substrate orientation on the electronic and optical properties of InAs/ GaAs quantum dots1, VLADAN MLINAR, FRANCOIS PEETERS, Department of Physics, University of Antwerp — Variation of the electronic and optical properties of InAs/GaAs quantum dots (QD) as a function of the substrate orientation is studied in the framework of 3D eight-band k.p model. The QD transition energies are obtained for high index surfaces [11k], where k = 1, 2, 3 and are compared with [001]. We show that the QD size in the growth direction determines the degree of the influence of the substrate orientation, whereas the influence of the shape is of secondary importance. The effects of an external magnetic field parallel applied and perpendicular to the QD growth direction are analyzed taking into account the Zeeman effect and employing the gauge invariant discretization scheme. The available experimental data are successfully described by one of the optically active exciton states of the lowest lying exciton quartet. We also discuss the experimentally observed negative exciton diamagnetic shift for small values of the magnetic field: (1) for samples grown on a (001) substrate and magnetic field applied parallel to the growth direction, and (2) for samples grown on a (311) substrate and magnetic field applied parallel to the growth direction.

1This work was supported by the European Union Network of Excellence: SANDIE

4:54PM L43.00013 Self-assembled (In,Ga)As Quantum Posts on GaAs, JUN HE, University of California, Santa Barbara(UCSB), Department of Materials, Santa Barbara, CA 93106 USA, HUBERT KRENNER, UCSB, Department of Materials, Santa Barbara, CA 93106 USA, CRAIG PRYOR, University of Iowa, Department of Physics and Astronomy, Iowa City, IA 52242 USA, JINGPIN ZHANG, YUAN WU, UCSB, Department of Physics, Santa Barbara, CA 93106 USA, DAN ALLÈN, CHRIS MORRIS, MARK SHERWIN, UCSB, Department of Materials, Santa Barbara, CA 93106 USA, PIERRE PETROFF, UCSB, Department of Materials, Santa Barbara, CA 93106 USA, HUBERT KRENNER, UCSB, Department of Materials, Santa Barbara, CA 93106 USA, DAN ALLÈN, CHRIS MORRIS, MARK SHERWIN, UCSB, Department of Materials, Santa Barbara, CA 93106 USA — We demonstrate a method for the MBE growth of (In,Ga)As quantum posts (QPs). Its main axis is along the growth direction. They are dislocation free and have dimensions $\approx 20$ nm in width, $\approx 25$ nm in length, and $\approx 50$ nm in height controlled. The QD size in the growth direction determines the degree of the influence of the substrate orientation, whereas the influence of the shape is of secondary importance. The effects of an external magnetic field parallel applied and perpendicular to the QD growth direction are analyzed taking into account the Zeeman effect and employing the gauge invariant discretization scheme. The available experimental data are successfully described by one of the optically active exciton states of the lowest lying exciton quartet. We also discuss the experimentally observed negative exciton diamagnetic shift for small values of the magnetic field: (1) for samples grown on a (001) substrate and magnetic field applied parallel to the growth direction, and (2) for samples grown on a (311) substrate and magnetic field applied parallel to the growth direction.

5:06PM L43.00014 Measurements of the bandgap of wurtzite InAs$_{1-x}$P$_x$ nanowires using photocurrent spectroscopy, J TRAGARO, A.I. PERSSON, Solid State Physics, Lund University, Sweden. We report measurements of the bandgap of InAs$_{1-x}$P$_x$ nanowires with wurtzite crystal structure as a function of the composition. The bandgap was measured using photocurrent spectroscopy (performed at 5 K) on single InAs nanowires with a centrally placed InAs$_{1-x}$P$_x$ segment, contacted at the InAs ends. The nanowires were grown with chemical beam epitaxy (CBE). The measured bandgap was larger than the bandgap of zincblende InAs$_{1-x}$P$_x$ by about 120 meV over the measured composition range, $0.15 < x < 0.5$. We attribute this increase to the fact that the crystal structure is wurtzite rather than zincblende. These measurements, combined with our previous measurements of the development of the conduction band off-set with composition [1] as determined by thermal activation measurements, allow us to determine the evolution of both the conduction and valence band off-sets with the InAs$_{1-x}$P$_x$ composition. [1] Persson et al. Nano Letters 6, 403 (2006)

5:18PM L43.00015 Magnetoplasmon excitations in Rashba spintronic quantum wires: Maxons, rotors, and negative energy dispersion, M.S. KUSHWAHA, University of Puebla — We investigate the plasmon excitations in a quasi-one-dimensional electron gas (Q1DEG) in the presence of a perpendicular magnetic field ($B$) and spin-orbit interaction (SOI) induced by the Rashba effect. The problem involves three length scales: $\ell_0 = \sqrt{h/m^*\omega}$, $\ell_\perp = \sqrt{h/m^*\omega}$, and $\ell = h^2/(2m^*\alpha)$ associated with, respectively, the confining potential, the magnetic field, and the Rashba SOI. The resulting Schrödinger-like equations satisfied by the wave function $\phi_{\perp}$ are two coupled equations, which cannot be solved in an explicit analytical form. However, the limit of a strong magnetic field ($\ell_\perp \ll \ell_0$) and $k_0 \ell < 1$ helps solve this set of coupled equations exactly. We derive and discuss the dispersion relations for charge-density excitations within the framework of Bohm-Pines’ RPA. The intrasubband and intersubband magnetoplasmons (MPs) in a Q1DEG are characterized by, respectively, the negative energy dispersion with increasing $B$ and the magnetoroton excitations. Here we scrutinize the effect of the SOI on these characteristics in depth. We observe that the SOI modifies drastically the behavior of both the intrasubband and intersubband MPs in the LW limit and renders them relatively more prone to the Landau damping in the SW limit. We discuss the dependence of the MPs energy on the propagation vector, the magnetic field, the 1D charge-density, and the Rashba parameter characterizing the SOI.

Tuesday, March 6, 2007 7:00PM - 8:00PM — Session M45 DCMP: DCMP Business Meeting Adam039;s Mark Hotel Plaza Court 6
which is under magnetic field successively being occupied by a spin-up and then a spin-down electron. The binding energy of the neutral $D$ below the conduction band edge. We can set the charge on the dopant by means of the gate electrode and observe the single and doubly charged donor state and have an active region as small as 50x60x35nm dimensional nano-scale devices consisting of a lithographically defined Si nanowire surrounded by a gate. They are fabricated on a Si-on-insulator substrate. In this talk we discuss the physics of transport and disorder, we discuss recent advances in silicon membranes that offer new ways to create quantum wells with lower disorder. Si membranes with thicknesses as thin as one hundred nanometers and lateral widths as large as a centimeter have been achieved. We discuss their application as hosts for quantum wells and as an enabling technology for the formation of Si/SiO2/Si multilayers in which all Si layers are single crystal. Work performed in collaboration with L.M. McGuire, C. Simmons, N. Shaji, K.A. Slinker, S. Goswami, L.J. Klein, W. Peng, M.M. Roberts, J.O. Chu, R. Joynt, M. Friesen, S.N. Coppersmith, R. Blick, M.G. Lagally, and D.E. Savage.

9:12AM N1.00003 Single-dopant spectroscopy in triple-gate nano MOSFETs 1, SVEN ROGGE, Kavli Institute of NanoScience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands — In this talk we discuss the physics of transport through a single dopant atom in a semiconductor matrix to which we have spectroscopic access in a prototype silicon MOSFET. These FinFETs are three dimensional nano-scale devices consisting of a lithographically defined Si nanowire surrounded by a gate. They are fabricated on a Si-on-insulator substrate and have an active region as small as 50x60x35nm. The electronic states of the dopant appear as resonances in the low temperature conductance at energies below the conduction band edge. We can set the charge on the dopant by means of the gate electrode and observe the single and doubly charged donor state which is under magnetic field successively being occupied by a spin-up and then a spin-down electron. The binding energy of the neutral $D^{-}$ state is consistent with that of an arsenic donor. The $D^{-}$ state with two electrons shows a reduced charging energy compared to bulk Si due to the electrostatic coupling with electrodes. The level spectrum of the dopant exhibits a large separation of the ground state from excited states but is not bulk-like. This is also due to the close proximity to the gate which leads to a strong electric field and the formation of a second well close to the interface that overlaps with the donor well. The manipulation of the dopant wavefunction by an electric field (Stark effect) is a key element in Si quantum electronics, e.g. the solid-state quantum computer. We discuss the level spectrum of this gated $D^{-}$ system for different field strengths up to 50 MV/m and relate it to theory. At these high fields the charge still remains localized but shows a strongly altered level spectrum. Recent references: H. Sellier et al., Transport Spectroscopy of a Single Dopant in a Gated Silicon Nanowire, PRL 97, 206805 (2006) and H. Sellier et al., Sub-threshold channels at the edges of nanoscale triple-gate silicon transistors, cond-mat/0603430

9:48AM N1.00004 Coherent electron spin transport and fault-tolerant semiconductor-based quantum computer architectures.1, Lloyd Hollenberg, Centre for Quantum Computer Technology, School of Physics, University of Melbourne — The recent progress in single atom fabrication techniques for discrete gated donor systems in semiconductors offer new opportunities for coherent quantum technology applications. We review a new scheme for coherent electron spin transport by adiabatic passage (CTAP) particularly suited to atomic and solid-state systems. In a semiconductor implementation, CTAP based transport is a highly robust mechanism for shuttling electron spin states coherently along pathways defined by ionised donors spaced 20-30 nm apart. Such novel discrete transport of electrons may lead to new applications in semiconductor technology, however, as a transport mechanism for spin-encoded quantum information it is an essential development for the successful design of a strongly scalable quantum computer architecture. Using phosphorous donor electron spins in silicon as a model system, the tunnelling rates, transfer times, and effects of decoherence are calculated. The introduction of electron spin transport leads to a scalable 2D quantum computer architecture for Si:P with spatially separated interaction, storage and readout regions and incorporates non-nearest-neighbour interactions between qubits. The transport rails which provide these non-local interactions, also provide alternative pathways to avoid non-functioning regions. The fault-tolerant operation of such an architecture using CTAP for qubit transport is considered in detail.

1 This work was supported by the Australian Research Council, the Australian Government, the US National Security Agency (NSA), Advanced Research and Development Activity (ARDA), and the Army Research Office (ARO) under contract number W911NF-04-1-0290.
8:00AM N2.00001 Superconducting qubits on the way to a quantum processor\textsuperscript{3}. FRANK WILHELM, IQC and Physics Department, University of Waterloo, 200 University Ave W, Waterloo, ON, N2L 3G1, Canada — Experimental research on superconducting qubits has seen an enormous progress in recent years. About 10 years after its first theoretical proposals, experiments have demonstrated the necessary building blocks for the exploration of quantum information along several avenues: Single qubit-rotations, long coherence times, high-fidelity non demolition readout, two-qubit interactions and gates, coupling to delocalized qubit modes. With this progress, analogies to other qubit candidates such as magnetic resonance systems, atomic, and optical systems are evident, but we also see the specific strengths of superconducting qubits play out - in situ tunable qubit-qubit coupling, strong coupling between qubits and the quantized electromagnetic field, strong intrinsic nonlinearity, and the possibility to fabricate large circuits. Most of these achievements will be discussed later in the session. I will give an introduction to superconducting qubits in the perspective of quantum information processing \cite{1} accessible to outsiders in the field. I will put the different elements of the session in the perspective of an actual scalable architecture which allows for fault-tolerant quantum computation \cite{1, 2}. In order to make further progress in direction, the fidelities of quantum operations need to be improved. I will discuss the crucial topic of understanding and further supressing noise from material defects in these systems, which can influence both the phase and bit-flip error rate \cite{3, 4}. I will show, how optimal control theory can help to find fast and high-fidelity shaped pulses for superconducting qubits, even though they, other than spin $1/2$ systems, have relatively close leakage levels outside the qubit manfold \cite{5, 6}. This technique also allows to optimize pulses in the presence of telegraph noise \cite{6}. Finally, I will describe how the strong nonlinearity of Josephson circuit can be used for the generation of single microwave photons \cite{7} and lead to a nonlinear generalization of cavity quantum electrodynamics effects \cite{8}.

\begin{thebibliography}{9}
\bibitem{2} A.G. Fowler, W. Thompson, Z. Yan, A.H. Majedi, and F.K. Wilhelm, in preparation
\bibitem{5} P. Rebentrost, I. Serban, T. Schulte-Herbruggen, and F.K. Wilhelm, in preparation
\bibitem{7} I. Serban, E. Solano, F.K. Wilhelm, cond-mat/0606734
\bibitem{8} Work supported in parts by the DFG through SFB 631, the EU through EuroQIP, NSERC Discovery Grants, and the University of Waterloo
\end{thebibliography}

8:36AM N2.00002 Solid State Qubits with Current-Controlled Coupling. TRAVIS HIME, University of California, Berkeley — The ability to switch the coupling between quantum bits (qubits) on and off is essential for implementing many quantum computing algorithms. We have demonstrated such control with two, three-junction flux qubits coupled together via their mutual inductances and via the dc SQUID (Superconducting Quantum Interference Device) that reads out their magnetic flux states. The flux in each qubit was controlled by an on-chip loop, and the chip was surrounded by a superconducting cavity that eliminates fluctuations in the ambient magnetic field. By applying microwave radiation to the device, we observed resonant absorption in each of the qubits when the level splitting in the qubit matched the energy of the microwave photons. With the qubits biased at the same frequency, the interaction produced an avoided crossing in their energy spectrum. At the avoided crossing transitions to the first excited state were suppressed and transitions to the second excited state enhanced, indicating formation of singlet and triplet states in the coupled-qubit system. The observed peak amplitudes were consistent with calculated matrix elements. When both qubits were biased at their degeneracy points, a level repulsion was observed in the energy spectrum. A bias current applied to the SQUID in the zero-voltage state prior to measurement induced a change in its dynamic inductance, reducing the coupling energy controllably to zero and even reversing its sign. The dependence of the splitting on the bias current was in good agreement with predictions. This work was performed in collaboration with P.A. Reichardt, B.L.T. Plourde, T.L. Robertson, C.-E. Wu, A.V. Ustinov, and John Clarke, and supported by NSF, AFOSR, ARO and ARDA.

9:12AM N2.00003 Measurement and Generation of Single Photons in a Circuit. ANDREW HOUCK, Yale University — I will describe the measurement and generation of single photons in a circuit quantum electrodynamics system. A one-dimensional transmission line cavity realizing well-defined microwave linear photon modes is coupled to a Cooper-pair box qubit. The qubit-photon coupling is exploited to realize a quantum non-demolition measurement of the qubit state by the photons, resulting in high visibility and long coherence times. The reverse measurement can also be performed: the qubit can be used to measure the number of photons in the cavity. In this case, the qubit transition is resolved into separate spectral lines for each photon number, leading to a photon statistics analyzer. The same interaction can also be used to convert qubit states into a flying qubit consisting of superpositions of photon states, and to generate single microwave photons on demand, enabling a full range of quantum optics experiments. Work done in collaboration with D.J. Schuster, A. Wallraff, A. Blais, J. Schreier, L. Frunzio, J.A. Gambetta, J. Koch, J. Majer, B. Johnson, J. Chow, T. Yu, M. Devoret, S.M. Girvin, R.J. Schoelkopf.

9:48AM N2.00004 Direct Measurement of the Entanglement of Two Superconducting Qubits via State Tomography. MATTHIAS STEFFEN, UCSB, IBM — The Josephson phase qubit can be thought of as an electrical "atom" whose resonance frequency can be tuned via an external control bias. Owing to its potential compatibility with conventional integrated circuit fabrication techniques, this system is a promising candidate for a scalable architecture for a quantum computer. Currently, the critical path towards a real device consists of understanding all sources of decoherence that destroy the fragile quantum states. Recently, dielectric loss was identified as the main source of decoherence for phase qubits. By employing techniques to minimize dielectric loss we improved the performance of our quantum bit, which enabled us to show quantum-mechanical entanglement between two phase qubits and identify the generation of a Bell state with a fidelity of up to 0.87, still limited by decoherence effects. We detail the experiment and outline further progress on reducing dielectric loss, leading to an improvement of the measured energy relaxation time by a factor of five. We also identified other insulating materials which should improve the energy relaxation time by an additional factor of two, resulting in overall coherence times of about one microsecond.

10:24AM N2.00005 Flux qubits: quantum non demolition readout and controlled-not gate\textsuperscript{1}. HANS MOOUJ, Delft University of Technology — Superconducting flux qubits have of a loop with three Josephson junctions, biased at about half a flux quantum. Basic states have opposite persistent currents, readout is by inductive coupling to a SQUID magnetometer. The following results have been obtained in a bias flux regime where the qubit energy states closely resemble the current states. Coherence was significantly lower than for the best samples. A dispersive method for readout was developed, where the inductance of the SQUID is measured rather than the critical current. The SQUID together with an on-chip capacitance forms a nonlinear oscillator where the resonant frequency depends on the flux in the SQUID, in turn influenced by the qubit. For high driving, two oscillation modes exist with low and high amplitude with a hysteretic transition. A short microwave pulse is applied and the probability that the oscillator switches to the high-amplitude mode is determined. This readout method yields a fidelity of 87\% without any corrections for relaxation. We have performed series of two consecutive measurements on a qubit in various superposition states and correlations between the outcomes were determined. Between the first measurement and the second a Rabi pulse was applied. Results were consistent with fully projective measurement, with a quantum non demolition fidelity of 88\% without corrections. We have also studied a system of two permanently coupled flux qubits. For each qubit, the energy splitting is shifted by the other qubit to plus or minus 200 MHz. When a suitable pulse is applied to a target qubit, it acts as a pi-pulse when the control qubit is in one state, and does nothing in the opposite case. This controlled-not operation that consists of a single microwave pulse has been performed for arbitrary superposition states of the two qubits. We have determined the phase reliability of the operation as well as its amplitude response.

\textsuperscript{1}In collaboration with Adrian Lupascu (present address Ecole Normale Paris), Jelle Plantenberg, Thomas Picot, Pieter De Groot, and Kees Harmans, Delft University of Technology.
Titanium: A Technical Guide

Preliminary results indicate the DFT-based cluster approach determines solubility limits and transformation temperatures that are in good agreement with the Ti-V phase diagram must take into account structures based on both bcc and hcp lattices over the full V concentration range. With the cluster expansion the high-temperature bcc phase of Ti at lower temperatures, while minimizing the formation of intermetallic compounds [1]. Theoretical determination of the


8:12AM N7.00003 Strain-Rate Frequency Superposition (SRFS) - A rheological probe of structural relaxation in soft materials, HANS M. WYSS, Harvard University — The rheological properties of soft materials such as concentrated suspensions, emulsions, or foams often exhibit surprisingly universal linear and nonlinear features. Here we show that their linear and nonlinear viscoelastic responses can be unified in a single picture by considering the effect of the strain-rate amplitude on the structural relaxation of the material. We present a new approach to oscillatory rheology, which keeps the strain-rate amplitude fixed as the oscillation frequency is varied. This allows for a detailed study of the effects of strain rate on the structural relaxation of soft materials. Our data exhibits a characteristic scaling, which isolates the response due to structural relaxation, even when it occurs at frequencies too low to be accessible with standard techniques. Our approach is reminiscent of a technique called time-temperature superposition (TTS), when the TTS curves measured at different temperatures are shifted onto a single master curve that reflects the viscoelastic behavior in a dramatically extended range of frequencies. By analogy, we call our approach strain-rate frequency superposition (SRFS). Our experimental results show that nonlinear viscoelastic measurements contain useful information on the slow relaxation dynamics of soft materials. The data indicates that the yielding behavior of soft materials directly probes the structural relaxation process itself, shifted towards higher frequencies by an applied strain rate. This suggests that SRFS will provide new insight into the physical mechanisms that govern the viscoelastic response of a wide range of soft materials.

8:36AM N7.00002 Nonlinear structural dynamics in metal nanowires, J ´ERÔME B ¨URKI, University of Arizona — Most atoms in a metal nanowire are surface atoms with low coordination number. Classically, surface effects are expected to dominate their stability and structural dynamics, leading in particular to wire break-up due to the Rayleigh instability. On the other hand, long gold [1] and silver [2] nanocylinders have recently been observed using transmission electron microscopy, pointing to the presence of an additional stabilizing mechanism. Evidence of electron-shell filling effects [3] have been found in conductance histograms for various metals, suggesting that this mechanism comes from the transverse confinement of the electrons within the nanowire. Using the nanoscale free-electron model, a continuum model of the structural dynamics of simple-metal nanowires, I will discuss how the interplay of surface and electron-shell effects explains the stability and long lifetimes of nanowires, and favors the formation of kinks connecting cylindrical segments of the wire. A rich dynamics involving kink interactions and kink/antikink pair-creation and annihilation is uncovered, and is shown to discuss how the interplay of surface and electron-shell effects explains the stability and long lifetimes of nanowires, and favors the formation of kinks connecting cylindrical segments of the wire. A rich dynamics involving kink interactions and kink/antikink pair-creation and annihilation is uncovered, and is shown to explain the observed step-by-step thinning mechanism of Au nanowires [4].

Wednesday, March 7, 2007 8:00AM - 11:00AM — Session N11 DCMP: Structural and Magnetic Phase Transitions Colorado Convention Center Korbel 1F

8:00AM N11.00001 Ti-V alloy phase diagram: DFT-based cluster approach1, MICHAEL R. FELLINGER, JOHN W. WILKINS, The Ohio State University, DALLAS R. TRINKLE, University of Illinois-UC — V is an important alloying element for Ti since it stabilizes the high-temperature bcc phase of Ti at lower temperatures, while minimizing the formation of intermetallic compounds [1]. Theoretical determination of the Ti-V phase diagram must take into account structures based on both bcc and hcp lattices over the full V concentration range. With the cluster expansion formalism for alloys [2], DFT calculations determine the energies of all structures necessary for constructing the cluster expansion for the energetics of the alloy. Preliminary results indicate the DFT-based cluster approach determines solubility limits and transformation temperatures that are in good agreement with the experimental phase diagram [3].

1Supported in part by the DOE. We thank R. G. Hennig of Cornell U. for useful discussions.
8:12AM N11.00002 Phase Transition to Modulated Cubic Phase in AuZn alloy\textsuperscript{1}. S. M. SHAPIRO, Brookhaven National Laboratory, J. C. LASHLEY, Los Alamos National Laboratory, W. RATCLIFF, National Institute of Standards and Technology, D. J. THOMA, J. L. SMITH, Los Alamos National Laboratory — AuZn is believed to undergo a martensitic transition from a high-temperature cubic phase to a reported low-temperature trigonal phase around 60K. Specific heat studies revealed that the transition is second-order for the 50-50 alloy, and first-order for off-stoichiometric compositions. Elastic neutron diffraction studies on a single crystal of the 50-50 alloy showed the surprising result that the martensitic transformation is suppressed and new Bragg peaks appear at $q_{\text{in}} = (1/3,1/3,0)$, in a continuous manner. The low-temperature structure can be viewed as cubic with a 3-fold increase in the cell along the [110] direction, similar to what has been observed in premartensitic phases. Attempts to measure the phonon dispersion curves using inelastic x-ray scattering will also be discussed.

\textsuperscript{1}Work at BNL and LANL supported by US. DOE., Work at NIST supported by U.S. DOC

8:24AM N11.00003 Structural Studies on First-Order Structure Transitions in RPD$_2$Ga$_2$. ROBIN MACALUSO, University of Northern Colorado, L. CHAPON, E. GOREMYCHKIN, ISIS Facility, Rutherford Appleton Laboratory, R. OSBORN, J. MITCHELL, Argonne National Laboratory, B. RAINFORD, Southampton University — We have investigated the structure of RPD$_2$Ga$_2$ (R = La, Ce) compounds by neutron powder diffraction. For the first time, a first-order structural transition is observed at $T_t = 70$ K and $T_t = 125$ K for CePd$_2$Ga$_2$ and LaPd$_2$Ga$_2$, respectively. The high-temperature structure ($T > T_t$) for both compounds is the tetragonal CaBe$_2$Ge$_2$ structure with lattice parameters of $a = 4.4791(4)$ Å and $c = 9.8373(2)$ Å and $a = 4.83185(19)$ Å and $c = 10.7548(5)$ Å for LaPd$_2$Ga$_2$ and CePd$_2$Ga$_2$ at 305 K, respectively. Below $T_t$ the symmetry of both structures descends to an orthorhombic space group, Pmmn. Lattice parameters at 2 K are $a = 6.07032(3)$ Å, $b = 12.90921(6)$ Å, $c = 9.87899(5)$ Å and $a = 6.3996(4)$, $b = 11.9058(8)$, $c = 9.9291(7)$ for LaPd$_2$Ga$_2$ and CePd$_2$Ga$_2$. In this talk, evidence for the order of the structural transition will be presented and the low and high temperature structures will be discussed.

8:36AM N11.00004 High pressure phases of alkali ternary borohydrides. RAVHI KUMAR, HiPSEC, Department of Physics, University of Nevada Las Vegas, ANDREW CORNELIUS, HiPSEC, Dept. Physics, University of Nevada Las Vegas — In situ synchrotron x-ray diffraction experiments were carried out on MBH$_3$ (M = K and Rb) borohydrides at high pressures up to 26 GPa using diamond anvil cells. KBH$_4$ undergoes a structural transition at 4 GPa to a tetragonal phase from cubic and then to an orthorhombic phase around 7 GPa which are very similar to NaBH$_4$ presented earlier [1]. However, RbBH$_4$ shows, a direct transition from the ambient cubic to an orthorhombic phase around 7 GPa which are very similar to NaBH$_4$ investigated earlier [1]. In the cubic phase display a very flat band at the Fermi level. Thus the low temperature tetragonal distortion has been associated to a Jahn-Teller effect. Previous total energy calculations of the tetragonal distortion for TiH$_2$ and ZrH$_2$ correspond to a displacive mechanism, will also be explored.


8:48AM N11.00005 First-principles study of the Jahn-Teller distortion in transition metal dihydrides.\textsuperscript{1}. RAMIRO QUIJANO, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Mérida, México — The transition metal dihydrides TiH$_2$ and ZrH$_2$ present the fluorite structure (CaF$_2$) at high temperature but undergoes a tetragonal distortion with $c/a < 1$ at low temperature. Early electronic band structure calculations have shown that TiH$_2$ and ZrH$_2$ in the cubic phase display a very flat band at the Fermi level. Thus the low temperature tetragonal distortion has been associated to a Jahn-Teller effect. Previous total energy calculations of the tetragonal distortion for TiH$_2$ within the Density Functional Theory (DFT), find that the ground state correspond to a tetragonal structure with $c/a > 1$, in contradiction with the experimental observation ($c/a < 1$). In the present work, we have performed full-potential LAPW calculations using the Local Density Approximation (LDA) and the Generalized Gradient Approximation (GGA) for the exchange correlation functional energy. Special attention was paid to the convergence of the total-energy calculations, so that in TiH$_2$ the energy differences for a tetragonal distortion at constant volume are only fractions of 1 mRy. We find that the ground state of TiH$_2$ and ZrH$_2$ corresponds to a tetragonal distorted structures with $c/a < 1$, in agreement with the experimental observations. The same behavior is predicted for HfH$_2$. The electronic band structure of the three systems is analyzed in the context of the Jahn-Teller effect.

\textsuperscript{1}Research supported by CONACYT-México under Grant No. 43830

9:00AM N11.00006 Phonon-based Mechanisms for Structural Transformations in Pu. TURAB LOOKMAN, AVADH SAXENA, ROBERT ALBERS, Los Alamos National Laboratory — Plutonium undergoes a number of transformations that involve changes in unit cell shape and numbers of atoms. We focus on the fcc to monoclinic transformation, assuming a displacive mechanism, will also be explored.
9:36AM N11.00009 Time-domain thermoreflectance of FeRh across magnetic/structural phase transition. D.A. WALKO, J. WANG, Advanced Photon Source, Argonne National Laboratory, D.G. CAHILL, University of Illinois, Urbana-Champaign, J.-U. THIELE, E.E. FULLERTON, Hitachi Global Storage Technologies — As FeRh is heated above ~100º C, an antiferromagnetic to ferromagnetic phase transition is accompanied by an abrupt expansion in its lattice parameter of ~0.5%. This first-order phase transition has a large temperature hysteresis (often >20º). Ultrafast laser pulses have been shown to heat thin FeRh films through the phase transitions on a picosecond time scale. We have used time-domain thermoreflectance (TDTTR) in the temperature range 35 to 160º C to study FeRh films grown on MgO substrates. The TDTTR measurements were performed with a mode-locked Ti:Sapphire laser; the sample was slightly heated with the near-infrared pump beam, and small changes in the sample’s reflectivity were observed with the delayed probe beam using lock-in detection. We used TDTTR to measure the thermal conductance of the film/substrate interface. Additionally, the small temperature excursions produced in TDTTR allowed us to observe the transient behavior of FeRh at various temperatures across the phase transition. The reflectivity is affected by fast changes in the film’s optical properties and in its thickness, and we discuss the effects of hysteresis on the measurement. Work supported by U.S. Department of Energy.

9:48AM N11.00010 Thermodynamic and transport anisotropic properties of RVsb3 crystals1. ATHENA S. SEFAT, SERGEY L. BUD’KO, PAUL C. CANFIELD, Ames Laboratory, Department of Physics and Astronomy, Iowa State University, Ames, Iowa, 50011 — The RVsb3 series (R=La, Nd, Sm, Gd - Dy) offers the possibility of studying the magnetic ordering in materials with a single, crystallographically unique, rare-earth site. The anisotropic magnetization M(H, T), resistivity, and heat capacity C(T) results, on flux-grown crystals, will be presented. All of the compounds are metallic, and all, with the exceptions of non-magnetic LaVs3b3 and ferromagnetic CeVs3b3, show features typical of antiferromagnetic order below 10 K. For CeVs3b3, the easy axis of magnetization is parallel to c in the ordered state, whereas for the antiferromagnetic RVsb3 members of Pr, Nd, Tb, and Dy, the crystalline fields confine the spins close to the a-axis. Given that CeVs3b3 is a rare example of a Ce-based ferromagnet, we measured the pressure dependence of Tc up to 10 kbar and found it to increase at a rate of 0.14 K/kbar.

1Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. W-7405-ENG-82. This work was supported by the Director for Energy Research, Office of Basic Energy Sciences.

10:00AM N11.00011 X-ray resonant magnetic scattering study of the spin-flip transition in Gd3Ge4, LIZHI TAN, Iowa State University, SHIBABARTA NANDI, ANDREAS KREYSSIG, SHUANG JIA, ALAN GOLDMAN, ROBERT MCQUEENEY, PAUL CANFIELD, JONATHAN LANG, ZAHRIL ALAM, THOMAS LOGRASSO, DEBORAH SCLAGEL, VITALI PECHARSKY, KARL SCHNEIDNER, DEPARTMENT OF PHYSICS AND ASTRONOMY, IOWA STATE UNIVERSITY TEAM, ADVANCED PHOTOON SOURCE, ARGONNE NATIONAL LABORATORY COLLABORATION, AMES LABORATORY, USDIE COLLABORATION, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, IOWA STATE UNIVERSITY TEAM — Gd3Ge4 crystallizes in the orthorhombic space group Pnma. Below 127 K the Gd moments order antiferromagnetically in a layered structure with a magnetic unit cell same as the chemical unit cell. The ferromagnetic Gd-rich slabs are stacked antiferromagnetically along b-axis. The magnetic moments are primarily aligned along the c-axis. X-ray resonant magnetic scattering was used to study a fully reversible spin-flip transition in a single crystal Gd3Ge4 and to elucidate details of the magnetic structure in the spin-flip phase. The Gd moments at the three Wyckoff sites flop from c-axis antiferromagnetically aligned to a-axis antiferromagnetically aligned in a critical field Haf = 9 kOe applied along c-axis at T = 10 K. The magnetic space group changes from Pnma’a to Pnma’m’a at all three sites.

10:12AM N11.00012 Pressure-Dependent Magnetization Studies of Two Rare Earth-Based Intermetallic Systems1, R.P. GUERTIN, Tufts Univ., E.S. CHOI, Florida State Univ., B. ANDRAKA, C.R. ROTUNDU, Univ. of Florida, W. MCCALLUM, Y. JANSSON, Iowa State Univ. — Pressure dependent magnetization studies have been performed on two rare earth-based ternary intermetallic systems, R2Co3N5, where R=Gd, Dy and Pr, and Pr3Ni2Si5, the n=2 member of the Pr(n+1)(n+2)Ni(n)(n+1)2Si(n) family. The pressure dependence of the magnetization was measured for 2<T<300 K, 0<H<9 T and hydrostatic pressures 0<P<8 kbar using a vibrating sample magnetometer. For the R2Co3N5 system, R=Dy and Gd order antiferromagnetically at TN = 17.0 and 34.5 K, respectively and dTN/dP = +0.1 K/kbar for R=Dy and +0.4 K/kbar for R=Gd. Pr3Ni2Si5 is a van Vleck paramagnet, indicating a crystalline electric field (CEF) singlet ground state. For Pr3Ni2Si5, the Curie temperature (TC<35.0 K) and the saturation magnetization (1.5µB/Pr) decrease non-linearly with increasing pressure, consistent with a pressure-induced increase in the CEF splitting. The Pr4+ ground state is presumably a singlet, as the local Pr symmetry is very low. Preliminary high field VSM data suggest that a CEF level crossing occurs at 10.5 T where magnetization increases sharply to above 3.0 µB/Pr.

1Supported by NHMFL Visiting Scientist Program #43

10:24AM N11.00013 The equivalency between hydrostatic pressure and Si doping in the giant magnetocaloric compound Gd3(Si1−xGex)4 studied by X-Ray Magnetic Circular Dichroism. Y.C. TSENG, Northwestern University, D. HASKEL, J. LANG, S. SINOGEIKIN, Argonne National Laboratory, YA. MUDRYK, V.K. PECHARSKY, Ames Laboratory, K. SCHNEIDNER JR., Materials and Engineering Physics, Ames Laboratory, ADVANCED PHOTOON SOURCE, ARGONNE NATIONAL LABORATORY COLLABORATION, MATERIALS AND ENGINEERING PHYSICS, AMES LABORATORY COLLABORATION — The effect of pressure (P<150 kbar) upon the magnetic properties of giant magnetocaloric material Gd3(Si1−xGex)4 (x=0.125, 0.5) was investigated by x-ray magnetic circular dichroism measurements in a diamond anvil cell. The ferromagnetic Curie temperature, TC, increases linearly with pressure albeit with different slopes dTC/dP=+0.1 K/kbar for R=Dy and +0.4 K/kbar for R=Gd. Pr3Ni2Si5, the van Vleck paramagnet, indicates a crystalline electric field (CEF) singlet ground state. For Pr3Ni2Si5, the Curie temperature (TC<35.0 K) and the saturation magnetization (1.5µB/Pr) decrease non-linearly with increasing pressure, consistent with a pressure-induced increase in the CEF splitting. The Pr4+ ground state is presumably a singlet, as the local Pr symmetry is very low. Preliminary high field VSM data suggest that a CEF level crossing occurs at 10.5 T where magnetization increases sharply to above 3.0 µB/Pr.

1Supported by NHMFL Visiting Scientist Program #43

10:36AM N11.00014 Fluctuation induced first-order phase transitions in a dipolar Ising ferromagnetic slab. RAFAEL M. FERNANDES, Brazilian Synchrotron Light Laboratory and IFGW, Unicamp, Brazil, HARRY WESTFAHL JR., Brazilian Synchrotron Light Laboratory — We investigate the size effects on the magnetic phase diagram of an Ising ferromagnetic slab with finite width and finite thickness in which two interactions compete: the short-range strong exchange interaction and the long-range weak dipolar one. We show that the homogeneous ordered state is unstable towards the formation of a modulated phase and that thermal fluctuations induce a first-order Brazovskii transition. By considering striped and bubble modulated configurations, we show that the first has a lower energy and a higher spinodal limit and that in the most stable ordered phase the order parameter is modulated along the limited direction but uniform along the unlimited one. This effect is shown to be a consequence of finite lengths and of Dirichlet boundary conditions in a system with competing interactions. Applications of this model to the domain structure of thin films are discussed, specially for the case of MnAs:GaAs thin films, for which qualitative behaviors of the number of domains and of the mean value of modulation as functions of the temperature are outlined.
The mechanism of Fermi level pinning/unpinning at high k Oxide/GaAs interface. M.L. HUANG, W.C. LEE, P. CHANG, T.D. LIN, Y.J. LEE, M. HONG, Dep. of Materials Science and Engineering, National Tsing Hua Univ., Hsinchu, Taiwan, J. KWO, Dep. of Physics, National Tsing Hua Univ., Hsinchu, Taiwan — Unpinning of Fermi level at oxide/GaAs interface is the one of the key issues of realizing GaAs-based III-V metal-oxide-semiconductor field-effect-transistors (MOSFETs) for high-speed and high power applications due to inherent advantages of high electron mobility, semi-insulating substrates, and high breakdown fields. In this study several important high dielectric constant materials, Al2O3, HfO2, Ga2O3(Gd2O3) and Y2O3, were in-situ deposited on GaAs(001), and exhibited the different Fermi level pinning/unpinning behavior of current-capacitance (C-V) characteristics. In order to correlate the relationship between the oxide/GaAs interfacial structure and their electrical behavior, in-situ XPS analysis was conducted shortly after nano high k oxides were deposited on GaAs. Our studies suggest that Fermi level unpinning in the oxide/GaAs hetero-structure is attributed to the exclusion of the As-As and the As-O bonding during the initial interfacial formation.

8:12AM N20.00002 MOS Ge Diodes Based on High k Gate Dielectrics Grown by MBE and ALD. KUN YU LEE, W.C. LEE, T.D. LIN, C.S. LEE, Y.C. CHANG, Y.J. LEE, M.L. HUANG, Y.D. WU, M. HONG, Department of Materials Science and Engineering, NTU, Taiwan, J. KWO, Department of Physics, NTU, Taiwan — Germanium-based CMOS technology is gaining importance due to its high carrier mobility. In this work high k gate-dielectrics, Al2O3, HfO2, Y2O3 and Ga2O3(Gd2O3) grown by MBE and ALD were investigated as passivation layers on n-type Ge(100). Thermal stability of the MOS diodes was examined during various anneals. Prior to dielectric depositions surface pretreatments were applied to reduce the unwanted GeO2 interfacial layer, and to improve electrical properties. Frequency dispersion of C-V curves was reduced by using a 350°C precooling process, compared to the sample without precooling. The leakage current density of ALD grown HfO2 (6.8nm) is \(4 \times 10^{-7} \text{ A/cm}^2\) with \(k\) of 10.5. The improved CV curve was attributed to less GeO2 formed at substrate and oxide interface, as confirmed by XPS analysis. However, with higher cleaning temperature over 400°C, the CV curves showed additional inversion capacitance, possibly due to minority carriers from defect states near the interface.

8:24AM N20.00003 Inelastic Electron Tunneling Spectroscopy of Silicon Based MOS Diode with High Permittivity Gate Dielectrics. SYUANLONG YOU — Inelastic electron tunneling spectroscopy (IETS) has been known as a powerful technique for detecting the molecular vibrations in the spectra. This technique was also applied to the study of the silicon MOS to reveal the information of electrode phonons, dielectric phonons, chemical bonding, and trap states in MOS structure. In this work IET spectra of silicon MOS diode with SiO2, high k HfO2, and YDH (HFO2 doped with Y2O3) as gate dielectrics were investigated. The gate bias dependence of the IET spectrum enables us to ascribe the vibration mode adjacent to the metal gate interface, or to the silicon substrate interface. We show variations of the IET spectrum with respect to Y2O3 doping and annealing conditions of the dielectrics, and compare with reported data of infrared, Raman, and XPS. We also present the changes in IET spectra as induced by electrical stress that eventually leads to soft-breakdown in the dielectrics.

8:36AM N20.00004 MBE and ALD grown High k Dielectrics Gate Stacks on GaN. Y.C. CHANG, K.Y. LEE, W.C. LEE, T.D. LIN, Y.J. LEE, M.L. HUANG, M. HONG, Dept. of Materials Science and Engineering, National Tsing Hua Univ., Taiwan, J. KWO, Dept. of Physics, National Tsing Hua Univ., Taiwan, Y.H. WANG, Dept. of Electrical Engineering, National Cheng-Kung Univ., Taiwan — III-nitride compound semiconductors are attractive for high-temperature and high-power MOSFET applications due to their intrinsic properties of wide band gap, high breakdown field, and high saturation velocity under high fields. In this work GaN-based high k MOS diodes were fabricated using MBE-grown Ga2O3(Gd2O3), MBE-grown HfO2, and ALD-grown HfO2 as the gate dielectrics with dielectric constants of 14.7, 17.4 and 16.5, respectively. All MOS diodes exhibited low leakage (<10^-6 A/cm² at Vf=+1) and well behaved capacitance-voltage curves with a low interfacial density of states of ~10^11 cm^-2eV^-1. Energy-band diagrams of the MOS structures have been determined by extracting valence-band offset (ΔEᵥ) from HR-XPS and with the bandgaps of the oxides. For example, the ALD-grown HfO2-GaN at the interfaces approximately ΔEᵥ and ΔEᵥ of 1.2 eV and 1.1 eV, respectively.

8:48AM N20.00005 Spectroscopic Study of Band Alignment in Alternative High-k MOS Dielectric Stacks. E. BERSCH, S. RANGAN, E. GARFUNKEL, R.A. BARTYNSKI, Rutgers University — The study of high-k dielectrics and metal gate electrodes is critical to next generation MOSFETs. We have measured the band offsets of alternative MOS stacks using photoemission and inverse photoemission in the same chamber as well as synchrotron photoemission. At Rutgers, we have measured the valence and conduction band densities of states (DOS) and edges with UV photoemission and inverse photoemission, respectively, in situ. Using synchrotron photoemission we have measured the core level positions as well as the valence band DOS of clean and chemicalized/doped Si systems. The measurement of the chemical shifts of the core levels upon metallization enables us to evaluate the conduction band offset at the metal/dielectric interface. For Hf(6s)Si(1x)O(2), we find the conduction band offset (CBO) does not change as x is varied from 1 to 0.8, but the valence band offset increases by 0.4 eV. Titanium, aluminum and ruthenium were chosen as gate metals because of their prospective use as low and high workfunction metals in dual metal gate MOSFETs. We measured the CBO for Ti, Al and Ru/Hf(6s)Si(1x)O(2) interfaces and found barriers involving Ti and Ru to be in good agreement with the interface gap state model, whereas the barrier involving Al deviated substantially from it due to the formation of an AlO(X) layer at the interface.
9:00AM N20.00006 First-principles study of direct electron tunneling through ultra-thin SiO$_2$ layers, JOONG KANG, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, South Korea, Y.-H. KIM, Department of Materials Science and Engineering, Seoul University, South Korea — As the size of metal-oxide-semiconductor devices is scaled down to the sub-10 nm regime, the thickness of SiO$_2$ insulating layers reaches the range of 1-2 nm. Then, gate leakage current is unavoidable due to direct tunneling of electrons. In this work, we study the electron tunneling current through thin gate oxide layers for various Si(100)/SiO$_2$ interface models, which have different oxide thicknesses and crystal phases. We use a combined approach of the local-density-functional approximation and the matrix Green’s function method. We test oxide layers in the α-quartz, tridymite, and amorphous structures, which are sandwiched between two Si(100) electrodes. We find that Si induced gap states result from a decay of the silicon valence (conduction) band wave functions into the oxide region. The gate leakage current between two p+ Si electrodes is exponentially reduced as the oxide thickness increases, with the almost same decay rate of ~1 decade/0.2 nm, regardless of the structure of oxide layers. We also find that the gate leakage current is affected by introducing interface roughness and oxygen vacancies in the oxide.

9:12AM N20.00007 Search for Sub lattice Disorder in CaCu$_2$Ti$_2$O$_{12}$, KEVIN STONE, JAE-HYUK HER, PETER STEPHENS, Stony Brook University, JONATHAN HANSON, HAIDING MO, CHRISTIE NELSON, LIJUN WU, YIMEI ZHU, Brookhaven National Laboratory — One of the proposed mechanisms for the Internal Barrier Dielectric Capacitance believed to be responsible for the giant dielectric response of the perovskite material CaCu$_2$Ti$_2$O$_{12}$ is that of sub lattice disorder on the Ca and Cu sites. Such disorder should have measurable affects on both the intensity and shape of the Bragg peaks of different symmetries. We investigate the possible existence of such disorder through high resolution charge density maps, based on a large dataset of x-ray and electron diffraction integrated intensity measurements, and, separately, peak shape measurements on a restricted set of reflections. Supported by the U.S. Department of Energy.

9:24AM N20.00008 Extrinsic Mechanisms for the Giant Dielectric Constant in CaCu$_2$Ti$_2$O$_{12}$: A Low-Temperature Specific-Heat Study, C.P. SUN, H.D. YANG, JIANJUN LIU, W.N. MEI, J.-Y. LIN, CHUN-GANG DUAN, NATIONAL SUN YAT-SEN UNIVERSITY, TAIWAN TEAM, UNIVERSITY OF NEBRASKA AT OMAHA, USA TEAM, NATIONAL CHIAO-TUNG UNIVERSITY, TAIWAN TEAM, UNIVERSITY OF NEBRASKA-LINCOLN, USA TEAM — Low-temperature specific-heat study has been performed on the insulating giant dielectric constant material CaCu$_2$Ti$_2$O$_{12}$. Analyzing the specific heat data in the very low-temperature range (0.6 to 1.5 K) and moderately low-temperature range (1.5 to 5 K), we noticed significant contributions originated from the linear and Einstein terms, we attributed as the low-lying elementary excitations due to lattice vibrations occurred at the grain boundaries and induced by local defects. These findings correlate well with the core-shell model deduced from the earlier experiments, and offer explanation to the extrinsic mechanisms of the giant dielectric constants at both low ($10^{-5}$ Hz) and high frequency ($10^7$ to $10^{10}$ Hz) regions.

9:36AM N20.00009 Fabrication and properties of TiO$_2$ cluster films, XIAOHUI WEI, Y.F. XU, Z SUN, RALPH SKOMSKI, D.J. SELLMYER, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska — Recently much interest has been directed toward nanostructured pure and doped semiconductors for their interesting dielectric, optical and magnetic properties and potential applications in spintronic devices. In this study a gas-condensation cluster-deposition system was used to make cluster-assembled films. Ti and TiO$_2$ targets were used to prepare Ti and TiO$_2$ cluster assembled films. The Ti and TiO$_2$clusters were examined by TEM to determine their size and size distribution. Films were scanned by AFM to see their surface morphology and examined by XRD to see their structural evolution with annealing temperature and annealing time. TEM revealed that the sizes of the Ti and TiO$_2$ clusters are 9 and 20 nm respectively. After annealing at 400 °C for an hour in oxygen, the Ti cluster films transform into pure polycrystalline rutile, which has a high dielectric constant, whereas the TiO$_2$ cluster films remain a mixture of anatase and rutile phases down to 400 °C annealing. The optical, magnetic and dielectric properties of the films will also be discussed. This work is sponsored by NSF-MRSEC,ONR and NCN.

9:48AM N20.00010 Second-harmonic generation measurements of porous low-k dielectric materials, JOANNA ATKIN, DAOHUA SONG, ROBERT LAIBOWITZ, Columbia University, EDUARD CARTIER, THOMAS SHAW, ROBERT ROSENBERG, IBM T. J. Watson Research Center, Yorktown Heights, NY 10598, TONY F. HEINZ, Columbia University, New York, NY 10027 — Low-k dielectric materials based on porous carbon-doped oxides, with relative dielectric constants as low as 2.1, are widely used in the microelectronics industry. Knowledge of these materials’ basic electronic properties, such as energy gaps, barrier heights, and trap states, is essential for developing an understanding of their electrical leakage and stability characteristics. In this paper, we present the results of measurements of optical second-harmonic generation (SHG) from thin films of the low-k material deposited on silicon. SHG measurements at low laser fluence probe the nature of interfacial trap states. At higher fluence, multiphoton charge injection is produced by the femtosecond laser pulses and yields a time dependence of the SHG signal. Analysis of these measurements provides information about barrier heights. The results of these non-contact optical measurements will be compared with C-V characterization of the dielectric films.

1Supported by the Semiconductor Research Corporation

10:00AM N20.00011 First-principles calculations for the elastic properties of superhard TiN/Si$_3$N$_4$ superlattices, SANWU WANG, Department of Physics and Engineering Physics, University of Tulsa, Tulsa, OK 74104, Y.G. SHEN, Department of Manufacturing Engineering and Engineering Management, City University of Hong Kong, Hong Kong, S.T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235 — We report first-principles density-functional calculations for the atomic structures, the electronic properties, and the elastic properties of superlattices containing nano-scale crystalline TiN and thin layer of silicon nitride. We found that the elastic properties (bulk modulus, shear modulus, and elastic constants) are strongly dependent on the size of the components. Superlattices with TiN thickness smaller than 2.5 nm have far smaller values of bulk and shear moduli than bulk crystalline TiN, while ~3 nm TiN can make the superlattice have the elastic properties close to those of crystalline TiN. The results are helpful for optimization of the component size to achieve high values of both elastic properties and hardness.

1Supported by the National Science Foundation (CMS-0610057 and CMS-0645953) and the National Center for Supercomputing Applications (DMR060010N).

10:12AM N20.00012 ABSTRACT WITHDRAWN —

Wednesday, March 7, 2007 11:15AM - 2:15PM
Session P1 DCMP: Recent Advances in Magnetization Dynamics —
Colorado Convention Center Four Seasons 2-3
11:15 AM P1.00001 Imaging fast spin dynamics at the nanoscale with soft x-ray microscopy., PETER FISCHER, CXRO LBNL Berkeley CA 94720 — Nanoscale and multicomponent magnetic systems are attracting both fundamental interest and are widely used in technological applications such as high density magnetic storage and sensor devices. The challenge to modern magnetic microscopies is to image magnetic microstructures in such specimens with high spatial and time resolution and elemental specificity. Magnetic soft x-ray microscopy is a novel technique combining a spatial resolution down to currently 15nm, elemental sensitivity due to x-ray magnetic circular dichroism used as magnetic contrast mechanism and a sub-nm time resolution limited by the current time structure of the synchrotron radiation used as source for circularly polarized soft x-rays. We report on recent results and achievements in magnetic soft x-ray microscopy obtained at the full-field soft x-ray microscopy beamline 6.1.2 (XM-1) located at the Advanced Light Source in Berkeley CA. Magnetization reversal processes at the grain level in a nanogranular CoCrPt system were studied with 15nm spatial resolution to obtain insight into spin fluctuations on a fundamental length scale. The inherent elemental sensitivity of XMCD contrast allows e.g. in (coupled) multilayered magnetic systems to explore their microscopic magnetization reversal process with layer resolution. Spin dynamics in magnetic nanostructures can be addressed by a stroboscopic pump and probe scheme utilizing the inherent time structure of synchrotron radiation, where the pump is a fast electronic pulse launched into a waveguide structure to excite the spin dynamics of a magnetic nanoelement. Varying the delay time between the pump and the probing x-ray flash one can follow the time development of e.g. local spin and vortex dynamics and relaxation phenomena, but also spin-torque driven domain wall displacements with sub-nm time resolution. Current developments of X-ray optics aim to achieve better than 10nm spatial resolution. At upcoming high brilliant ultrast x-ray sources snapshots of spin dynamics with fs time resolution recorded with magnetic soft x-ray microscopy can be foreseen. Many thanks to D.-H. Kim, B. Mesler, W. Chao, R. Oert, E. Anderson, G. Meier, R. Eiselt, M. Bolte, M.-Y. Im, S.-C. Shin, S. Mangin, E. Fullerton.

1This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

11:51 AM P1.00002 The Spin Transfer Torque Critical Current in Magnetic Nanopillars, ANDREW KENT, Department of Physics, New York University — Spin transfer in magnetic nanopillar has become a major focus of experimental research since Slonczewski and Berger’s seminal theoretical work in 1996. A spin current has been demonstrated to switch the magnetization direction of a small magnet at a specific current density, as well as to induce microwave excitations. However, there are basic questions about the factors that control the critical current density for magnetization dynamics. For instance, in Slonczewski’s model, spin angular momentum transfer occurs at ferromagnetic-non-magnetic interfaces and competes with bulk magnetization damping. This model predicts a critical current that scales linearly with ferromagnet layer thickness and extrapolates to zero in the limit of zero thickness. In this talk I will present experiments on Co (10 nm) /Cu (10 nm) /Co (t) nanopillars in which the Co free-layer thickness, t, has been varied from 2 to 5 nm. The critical current has been studied at low-temperature as a function of applied magnetic field perpendicular to the plane of the layers. The critical current decreases linearly with decreasing free-layer thickness, but extrapolates to a finite critical current in the limit of zero thickness, while the junction magnetoresistance is independent of thickness [1]. The limiting current is in agreement with that expected due to a spin-pumping contribution to the magnetization damping. It is also consistent with our FMRI studies of Co films, which indicate an enhancement of the magnetization damping in ultra-thin (<4 nm thick) Co layers due to spin-pumping [2]. Finally, I will discuss more recent studies of nanopillars with Ni/Co multilayer free layers. In these experiments, the role of the magnetic easy plane anisotropy can be explored, as this anisotropy varies with the number of Ni/Co interfaces within a fixed film thickness [3].

1In collaboration with J. Z. Sun (IBM), W. Chen and J-M. Beaujour (NYU). Supported by NSF-DMR-0405620.

12:27 PM P1.00003 Very low damping in epitaxial Fe and Fe1-xVx films, BILL BAILEY, Columbia University — No abstract available.

1:03 PM P1.00004 Spin Momentum Transfer and Oersted Field Induce a Vortex Nano-Oscillator in Thin Ferromagnetic Film Devices, MARK HOEFER, National Institute of Standards and Technology — A nonlinear model of spin-wave excitation involving a point contact in a thin ferromagnetic film that includes the Oersted magnetic field contribution is presented. We consider the case of an external dc field applied perpendicular to the film plane. The two-dimensional vectorial model reduces to an exact one-dimensional equation of motion. Large-amplitude vortex modes are computed, which represent a fundamental shift in the geometrical understanding of spin transfer nano-oscillators. Odd symmetry forces the magnetization to be pinned in the center of the point contact. Using the spin transfer efficiency as a single fitting parameter, the calculated dependence of frequency on current and contact size is in good agreement with recent experimental data. These vortex states are geometrically very different from previously computed cylindrical modes that exhibit even symmetry when the Oersted field is ignored.

1:39 PM P1.00005 Fingerprinting Magnetic Nanostructures by First Order Reversal Curves, KAI LIU, University of California - Davis — Realistic systems of magnetic nanostructures inevitably have inhomogeneities, which are manifested in distributions of magnetic properties, mixed magnetic phases, different magnetization reversal mechanisms, etc. The first order reversal curve (FORC) method [1-3] is ideally suited for “fingerprinting” such systems, both qualitatively and quantitatively. Here we present recent FORC studies on a few technologically important systems. In arrays of Fe nanodots [4], as the dot size decreases from 67 to 52nm, we have observed a vortex state to single-domain transition. Despite subtle changes in the major hysteresis loops, striking differences are seen in the FORC diagrams. The FORC method also gives quantitative measures of the magnetic phase fractions and vortex nucleation and annihilation fields. Furthermore, with decreasing temperature, it is more difficult to nucleate vortices within the dots and the single domain phase fraction increases. In exchange spring magnets [3], we have investigated the reversibility of the soft and hard layers and the interlayer exchange coupling. In FeNi/polycrystalline-FePt films, the FeNi and FePt layers reverse in a continuous process via a vortex state. In Fe/polyxial-SmO films, the reversal proceeds by a reversible rotation of the Fe soft layer, followed by an irreversible switching of the SmCo hard layer. As the SmCo partially demagnetizes, the Fe layer still remains reversible, as revealed by second order reversal curves (SORC). The exchange coupling between the two layers can be extracted as a function of the SmCo demagnetization state. These results demonstrate that FORC is a powerful method for magnetization reversal studies, due to its capability of capturing magnetic inhomogeneities, sensitivity to irreversible switching, and the quantitative phase information it can extract. Work done in collaboration with J. E. Davies, R. K. Dumas, J. Olami, C. P. Li, I. V. Roshchin, I. K. Schuller, O. Hellwig, E. E. Fullerton, J. S. Jiang, S. D. Bader, J. Wu, C. Leighton, H. G. Katzgraber, C. R. Pike, R. T. Scalettar, G. T. Zimanyi, and K. L. Verosub.

3J. E. Davies, et al, PRB 70, 224434 (2004); APL 86, 262503 (2005); PRB 72, 134419 (2005).

Supported by NSF, ACS-PRF, Alfred P. Sloan Foundation, AFOSR, and DOE.

11:15AM P3.00001 From nano to micro: hierarchical ordering at the nanoscale1. EZEKIEL JOHNSTON-HALPERIN, Department of Physics, Ohio State University — The overall goal of controlling structural and electronic materials properties at nanometer length scales can be thought of as the intersection of two distinct but correlated challenges. The first is the synthesis/fabrication of individual nanoscale structures and the second is the arrangement of those structures into tailored nano- and micro-scale assemblies. Motivated by these twin challenges, the development of the superlattice nanowire pattern transfer (SNAP) technique has enabled the fabrication of highly ordered arrays of hundreds of nanowires (both metallic and semiconducting) at pitches down to 16 nm and aspect ratios up to 102. As a result of the hierarchical ordering of these assemblies (ranging from nanometer to micrometer length scales), it is possible to achieve electronic point-addressability within the arrays using traditional lithography. Further, iterative use of this technique to generate orthogonal nanowire arrays yields extremely dense crossbar circuits: with a bit density of ~ 0.5 TBit/in2 (1011 Bits/cm2) these structures approach crystallographic density. Both realized and potential applications of these structures ranging from ultra-dense electronic circuits to optical and electronic meta-materials will be discussed.

1Research funded by DARPA.

11:51AM P3.00002 Controlled formation of epitaxial III-V nanowires for device applications , THOMAS MARTENSSON, Solid State Physics, Lund University — For the realization of devices with dimensions on the 10 nm scale, there is today a great interest in the possible use of self-assembly as a tool. In this talk will be described the state-of-the-art in growth of epitaxially nucleated, vertically standing semiconductor nanowires made from III-V semiconductors, with high level of control of dimensions, position and structural properties. Such wires hold great promise for use in future electronics and photonics applications. Three key aspects will be specifically addressed, namely: (1) The combination of top-down and bottom-up processes in lithographically aided formation of nanowires. A concern from industry is that bottom up techniques should suffer from “fundamental placement problem[s], i.e. there is no practical and reliable way to precisely align and position them.” (Chau R., et al. Opportunities and challenges of III-V nanoelectronics for future high-speed, low-power logic applications. (2005)). One way to resolve this issue is lithography where individual nanowire site control with high precision can be achieved. Electron beam lithography has the advantage of being a flexible high-resolution method, whereas nanoimprint lithography offers great opportunities for up-scaling and high-throughput processing. (2) The successful growth of III-V nanowires on silicon, including designed heterostructures. The special nanowire geometry with tens of nanometer radius and very small nanowire / substrate interface, enables monolithic integration of high-performance III-V materials on silicon substrates. As an example, GaAsP heterostructure nanowires for photonic applications are discussed. Also the formation of InAs nanowires for high-speed and low-power-electronics directly on Si will be described. In the latter process, the use of foreign metal particles for wire growth is completely avoided, greatly reducing compatibility concerns between CMOS and nanowire technology. (3) Nanowire devices, such as field-effect transistors and light-emitting diodes will be discussed.

12:27PM P3.00003 Electron confinement and long-range interactions in 1-D atom chains1 . DANIEL T. PIERCE, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899-8412 — In nanostructures, when electrons are confined to reduced dimensions, the geometry of the confinement leads to the formation of quantized electronic states. In turn, these quantized states determine the energetic stability of a particular geometry. For systems that are self assembled, where thermodynamics and the cohesive energy can play a key role in the formation process, this interplay between the geometry of the confinement and the electronic states leads to the formation of nanostructures with "magical sizes." Gold deposited on Si(553) leads to self-assembly of 1-D atomic chains, which are broken into finite segments by defects. Scanning tunneling spectroscopy measurements of the differential conductance along the chains revealed quantized states in isolated segments with differentiated states forming over the end atoms. These "end states" are the zero-dimensional analogs of the two-dimensional states that occur at a crystal surface[1]. Scanning tunneling microscopy was used to investigate the distribution of chain lengths and the correlation between defects separating the chains. The length distribution is not that for random defects, but exhibits oscillations that indicate changes in the cohesive energy as a function of chain length. We observe two separate components of the interaction at the Fermi surface. The correlation function shows long-range correlations that extend beyond nearest-neighbor defects, indicating coupling between chains[2].

1Supported in part by the Office of Naval Research.

1:03PM P3.00004 Biologically templated synthesis of Co3O4/Au nanowires for flexible Li-ion batteries , ANGELA BELCHER, The Massachusetts Institute of Technology — No abstract available.

1:39PM P3.00005 Superconductivity in DNA templated metal nanowires , ALEXEY BEZRYADIN, The University of Illinois at Urbana Champaign — No abstract available.

Wednesday, March 7, 2007 11:15AM - 1:39PM –
Session P5 DCMP: Entanglement Entropy in Condensed Matter Physics Colorado Convention Center
Korbel 1A-1B

11:15AM P5.00001 Probing order beyond the Landau paradigm , MICHAEL LEVIN, Harvard University — For many years, it was thought that Landau’s theory of symmetry breaking could describe essentially all phases and phase transitions. Then, in 1982, the limitations of Landau theory were exposed in a dramatic way with the discovery of the fractional quantum Hall (FQH) effect. The FQH states contain a new kind of order - known as “topological order” - that is fundamentally beyond the Landau paradigm. Topological order cannot be understood using symmetry breaking, order parameters, or long range order. This poses an interesting theoretical problem: these states must contain some kind of structure that is responsible for their unusual physical properties. But what is this structure and how can we probe it without order parameters? In my talk, I will describe recent progress in answering this question. I will show that topological order is intimately connected with nonlocal quantum entanglement. I will introduce a new quantity - called “topological entropy” - that measures precisely this nonlocal entanglement.
11:51AM P5.00002 Universal contributions to entanglement entropy at critical points in two spatial dimensions
Joel Moore, UC Berkeley and Lawrence Berkeley National Laboratory — The entanglement entropy of a pure quantum state of a bipartite system A ⊗ B is defined as the von Neumann entropy of the reduced density matrix obtained by tracing over one of the two parts. Critical ground states of local Hamiltonians in one dimension have entanglement that diverges logarithmically in the subsystem size, with a universal coefficient that for conformally invariant critical points is related to the central charge of the conformal field theory. We find the entanglement entropy for a standard class of ∼ = 2 quantum critical points in two spatial dimensions with scale invariant ground state wave functions: in addition to a nonuniversal ‘area law’ contribution proportional to the size of the AB boundary, there is generally a universal logarithmically divergent correction. This logarithmic term is completely determined by the geometry of the partition into subsystems and the central charge of the field theory that describes the equal-time correlations of the critical wavefunction. Taken together with results on entanglement entropy in gapped, topologically ordered phases, these results indicate that even when the ‘area law’ correctly predicts the leading behavior of entanglement, universal subleading terms can reflect important properties of a quantum many-body system.

12:27PM P5.00003 Entanglement entropy of quantum-critical spin chains with strong randomness
Gil Refael, California Institute of Technology — For disorder-free critical quantum spin chains, the entanglement of a segment of N ≫ 1 spins with the remainder scales as log N, with a prefactor fixed by the central charge of the associated conformal field theory. The mean entanglement entropy of quantum spin chains with randomness follows the same logarithmic scaling, and provides a universal critical entropy, which is equivalent to the central charge in the pure case. In my talk I will explore the origin and derivation of the universal entanglement entropy of the random spin-1/2 Heisenberg model in the random-singlet phase, as well as that of the random spin-1 Heisenberg chain at the breakdown of its Haldane phase. The entanglement of these and related infinite-randomness fixed points makes it possible to speculate on possible extensions of the c-theorem of CFTs to the realm of systems with strong randomness.

1:03PM P5.00004 Entanglement and efficient simulation of many-body quantum systems
Guifre Vidal, University of Queensland — No abstract available.

11:15AM P10.00001 Effects of Rhenium doping on the high magnetic field versus temperature phase diagram of URu2Si2
Sonia Francool, Neil Harrison, Marcello Jaime, Scott Baily, Alex Lacerda, National High Magnetic Field Laboratory, Los Alamos National Laboratory, Nicholas Butcher, Brian Maple, University of California, San Diego — Magnetoresistance and magnetization measurements carried out in URu2−xRe2Si2 at low temperatures and high magnetic fields for x values of the rhenium doping between 0.01 and 0.10 enable us to investigate the robustness of the multiple ordered phases previously identified in URu2Si2 near the putative metamagnetic quantum critical point at fields around 37 ± 1 T. From the transport study, rhenium doping is shown to reduce considerably the elliptical region occupied by the hidden order phase in the (H, T) phase diagram and to shift to lower fields the broad magnetoresistivity maximum observed in the high temperature phase. In addition, the upper temperature limit at which the field-induced phase transitions are observed inside the metamagnetic crossover region in the magnetization curves decreases rapidly with increasing rhenium doping. All results tend to indicate that for x < 0.10 the dilute substitution of Re in place of Ru in URu2Si2, unlike Rh substitution, weaken the ordering in the vicinity of the putative quantum critical point.

11:27AM P10.00002 Field-induced Fermi surface reconstruction and adiabatic continuity between antiferromagnetism and hidden-order state in URu2Si2
Y.J. Jo, L. Balicas, C. Capan, K. Behnia, P. Lejay, J. Flouquet, J.A. Mydosh, P. Schlottmann, Florida State University — Shubnikov-de Haas oscillations at very low temperatures and high magnetic fields reveal an abrupt reconstruction of the Fermi surface within the hidden-order phase of URu2Si2. Taken together with reported Hall effect results, this implies an increase in the effective carrier density and suggests spectrum of itinerant quasiparticles. While hydrostatic pressure favors antiferromagnetism in detriment to the hidden-order state, we found that it has a modest effect on the complex H−T phase diagram. This suggests adiabatic continuity between the hidden-order and antiferromagnetism.

11:39AM P10.00003 Interplay between Fermi surface topology and ordering in URu2Si2 revealed through abrupt Hall coefficient changes
Seok Oh, Kee Hoan Kim, P. A. Sharma, N. Harrison, K. Jung, O. O. Bernal, Physics and Astronomy Department California State University, Los Angeles, CA 90032; D. E. MacLaughlin, Physics and Astronomy Department, University of California, Riverside, CA 92521; T. J. Gortenmulder, Kamerlingh Onnes Lab, 2300 RA, Leiden, The Netherlands, J. A. Mydosh, Institute of Physics 2, University of Cologne, Zuelicher Str. 77, 50937 Koeln, Germany — We present NMR data for an epoxy-potted random-powder sample of URu2Si2. We have followed the line shape from 280 K down to about 4 K and observed its changing features as functions of temperature and two values of the applied magnetic field strength (1 and 2 T). We will describe the effects of the hidden order (transition temperature TH ≈ 17.5 K) on the line shape and compare them with previous results in c-axis oriented samples and single crystals.

11:51AM P10.00004 NMR Study of Line Shape Effects Caused by the Hidden Order in a Random Powder of URu2Si2
S. Jungs, O. O. Bernal, Physics and Astronomy Department California State University, Los Angeles, CA 90032; D. E. MacLaughlin, Physics and Astronomy Department, University of California, Riverside, CA 92521; T. J. Gortenmulder, Kamerlingh Onnes Lab, 2300 RA, Leiden, The Netherlands, J. A. Mydosh, Institute of Physics 2, University of Cologne, Zuelicher Str. 77, 50937 Koeln, Germany — We present NMR data for an epoxy-potted random-powder sample of URu2Si2. We have followed the line shape from 280 K down to about 4 K and observed its changing features as functions of temperature and two values of the applied magnetic field strength (1 and 2 T). We will describe the effects of the hidden order (transition temperature TH ≈ 17.5 K) on the line shape and compare them with previous results in c-axis oriented samples and single crystals.

Work supported by NSF/DMR-0604015.
12:03PM P10.00005 Inelastic neutron scattering studies of itinerant spin excitations in URu2Si2 near the hidden order transition. JOHN JANIK, NHMFL/FSU, G. MACDOUGALL, G. LUKE, McMaster University, Y.-J. JO, L. BALICAS, NHMFL, Y. QIU, J. COPLEY, NIST, Z. YAMANI, B. BUYERS, CNBC, National Research Council. C. WIEBE, NHMFL/FSU. We performed extensive neutron scattering studies on the heavy fermion superconductor URu2Si2. Using the C5 triple axis spectrometer at Chalk River, we studied the spin excitations recently reported [C. R. Wiebe, J. A. Janik et al., Nature Physics] above and below the Tc transition. It has become clear from our previous work that these incommensurate itinerant spin excitations account for the entropy change into the hidden order (HO) state. This severely limits the possible theoretical scenarios on the ground state of the HO phase.

12:15PM P10.00006 The Evolution of the Hidden Order Phase in URu2−xRe2Si2 under Pressure. , J.R. JEFFRIES, N.P. BUCHT, B.T. YUKICH, M.B. MAPLE, University of California, San Diego. The heavy fermion compound URu2Si2 exhibits three distinct ordered states as a function of temperature and pressure: “hidden order” (HO), in which the order parameter has yet to be identified; antiferromagnetism (AFM), which seemingly develops out of the HO state at P ≤ 15 kbar; and superconductivity (SC), which exists at ambient pressure. While URu2Si2, the parent compound of the URu2−xRe2Si2 system, has been the subject of much scrutiny in the past several years, the nature of the HO phase is still uncertain. The evolution of the ordered phases as a function of pressure in the URu2−xRe2Si2 system could provide clues to or constraints on the elusive order parameter of this HO phase. To this end, oriented single crystal samples of URu2−xRe2Si2 with small values of x have been synthesized and investigated under nearly hydrostatic pressure via electrical resistivity measurements. While the SC in URu2−xRe2Si2 is rapidly suppressed with Re concentration, the HO phase persists up to x ≈ 0.1. The pressure dependence of the HO phase in this concentration range will be discussed along with possible consequences to the ordered states. This research was sponsored by the U.S. DOE under Research Grant No. DE-FG02-04ER46105 and by the U.S. NNSA under the Stewardship Science Academic Alliances program through DOE Research Grant No. DE-FG52-03NA00068.

12:27PM P10.00007 The Search for Quantum Criticality in the URu2−xRe2Si2 Phase Diagram. , N.P. BUCHT, J.R. JEFFRIES, B.T. YUKICH, T.A. SAYLES, J. PAGLIONE, P.-C. HO, M.B. MAPLE, Dept. of Physics and IPAPS, University of California, San Diego. It has been established that as Re is doped into polycrystalline URu2Si2, the superconducting transition temperature Tc shows a strong suppression in the Re concentration range of 0 ≤ x ≤ 0.6 and performed magnetization, electrical and thermal transport, and calorimetry measurements at low temperatures down to 0.1 K.

12:39PM P10.00008 Crystal fields, magnetoresistance, and superconductivity of Pr1−xLa0.5Os0.5Sb12. BOHDAN ANDRAKA, COSTEL R. ROTUNDU, MARTIN E. MCBRIARTY, University of Florida. Investigation of Pr1−xLa0.5Os0.5Sb12 in strong magnetic fields implies that crystalline electric field (CEF) energies of Pr are unchanged to at least x=0.2. CEF energies for x=0.4 are approximately 20% larger than for x=0.2 and increase further for x=0.67. Specific heat discontinuity at Tc and the upper critical field slope at Tc indicate that the strongest suppression of m* takes place between x=0 and x=0.3. High accuracy specific heat data obtained on a large crystal of x=0.67 exhibit significant deviations with respect to the Schottky specific heat corresponding to singlet-triplet excitations. Similar deviations are seen for other crystals with x>xcr. On the other hand, magnetoresistance of moderately and strongly dilute alloys is consistent with predictions for a singlet-triplet CEF model. Correlations between these measurements of CEF's and superconductivity of Pr1−xLa0.5Os0.5Sb12 will be discussed. Also, evidences against and for homogeneous coexistence of two superconducting transitions in the specific heat of pure PrOs4Sb12 will be presented and discussed.

12:51PM P10.00009 A comparison of the normal and superconducting state properties of Pr(OS1−xRu1−y)Sb12 and Pr1−xNd0.5Os0.5Sb12. P.-C. HO, T. YANAGISAWA, N.P. BUTCH, W.M. YUHASSZ, N.A. FREDERICK, M.B. MAPLE, Physics and IPAPS/UCSD. The evolution of unconventional superconductivity and the high field ordered phase (HFOP), the latter of which has been identified with antiferroquadrupolar order, in PrOs4Sb12 has been investigated in two pseudoternary systems, Pr(OS1−xRu1−y)Sb12 and Pr1−xNd0.5Os0.5Sb12. In the Pr(OS1−xRu1−y)Sb12 system, the superconducting transition temperature Tc is suppressed nearly linearly with x to a minimum at x = 0.6 from both end member compounds, the upper critical field Hc2 has an approximately linear dependence on T for x > 0.4, and the features related to the HFOP in the electrical resistivity disappear for x ≥ 0.1. On the other hand, in the Pr1−xNd0.5Os0.5Sb12 system, Tc and the Curie temperature θC are suppressed monotonically toward x = 0.55 from x = 0 and x = 1, respectively, no linear T dependence of Hc2 is observed, the HFOP persists up to at least x ∼ 0.45, and there is an indication of the coexistence of superconductivity and ferromagnetism for x ~ 0.45 according to specific heat measurements. In both systems, Hc2(T) is limited by the orbital motion of the electrons and the decrease of Tc with x from x = 0 is nearly the same.

1The research at UCSD is funded by U.S. DOE and NSF.

1:03PM P10.00010 The disordered ground state of quantum critical Ce(Ru1−xFe1/2)2Ge2. WOUTER MONTFROOIJ, JAGAT LAMSAL, University of Missouri, MEIŽGAN ARONSON, MARCUS BENNETT, University of Michigan, ANNE DE VISSER, HUANG YING KAI, NGUYEN THANH HUI, van der Waals-Zeeman Institute, MARK LUMSDEN, Oak Ridge National Laboratory, MOHANA YETHIRAJ, Bragg Institute ANSTO, YIMING QIU, National Institute of Standards and Technology. We present neutron scattering data that show that magnetic ordering in the vicinity of a quantum critical point is restricted to short length scales. Remarkably, the spatial extent of the magnetic correlations is independent of the inter- moment distances. We argue that our data on Ce[Ru1−xFe1/2]2Ge2 demonstrate that quantum fluctuations disorder the system and dilute the magnetic moments to such an extent that the response of the system is disorder dominated. Our observations naturally explain how E/T-scaling is possible in systems whose apparent dimensionality is above the upper critical dimension.

2The work was supported by the Missouri Research Board [RB-03-081], by the NSF [DMR-0405961 and DMR-0454672] and by the Dutch foundation FOM.
1:15PM P10.00011 Magnetic field tuning of the low temperature state in YbNiSi$_3$: magnetic field induced quantum criticality\textsuperscript{1}. MARCOS A. AVILA, TOSHIRO TAKABATAKE, Dept. of Quantum Matter, ADSM, Hiroshima University, Japan, SERGEY L. BUDKO, PAUL C. CANFIELD, Ames Laboratory and Dept. of Physics and Astronomy, Iowa State University, USA — We present detailed, low temperature, magnetoresistance and specific heat data from measurements on YbNiSi$_3$ in magnetic field applied along the easy magnetic axis, $H/||c$. Initially the antiferromagnetic ground state changes into a field-induced metamagnetic phase at $\sim 16$ kOe ($T \rightarrow 0$). On further increase of magnetic field, magnetic order is suppressed to below 0.4 K at $\sim 85$ kOe. The functional behavior of the resistivity and specific heat is discussed in comparison with that of the few other stoichiometric, heavy fermion compounds with established field-induced quantum criticality. 

\textsuperscript{1}Aames Laboratory is operated for the U. S. Department of Energy by Iowa State University under Contract No. W-7405-Eng.-82. This work was supported by the director for Energy Research, Office of Basic Energy Sciences.

1:27PM P10.00012 Thermal Transport in ZrZn$_2$: Probing the Marginal Fermi Liquid State. MICHAEL SUTHERLAND, R. SMITH, University of Cambridge, K. NORIAKI, Centre for Low Temperature Science, Tohoku University, Sendai, Japan, G.G. LONZARICH, University of Cincinnati, THOMAS MAIER, RANDY FISHMAN, Oak Ridge National Laboratory — We describe here the use of Density Matrix Renormalization Group and Matrix Product algorithms for highly scalable impurity solvers in cluster Dynamical Mean Field Theory. We present results on 2- and 4-site clusters for the Hubbard model.

1:39PM P10.00013 ABSTRACT HAS BEEN MOVED TO R1 —

Wednesday, March 7, 2007 11:15AM - 2:15PM —

Session P11 DCMP: Correlated Electrons: DMFT

11:15AM P11.00001 DMRG-Based Solvers for Cluster DMFT. IAN MCCulloch, RWTH-Aachen, OLIVIER PARCOLLET, CEA-Saclay, ADRIAN KLEINE, ULRICH SCHOLLWÖCK, RWTH-Aachen — We describe here the use of Density Matrix Renormalization Group and Matrix Product algorithms for highly scalable impurity solvers in cluster Dynamical Mean Field Theory. We present results on 2- and 4-site clusters for the Hubbard model.

11:27AM P11.00002 An Extended Dynamical Cluster Approximation for Local-Moment Systems. KARLIS MIKELSONS, University of Cincinnati, Oak Ridge National Laboratory, THOMAS MAIER, RANDY FISHMAN, Oak Ridge National Laboratory, MARK JARRELL, University of Cincinnati — We introduce an Extended Dynamical Cluster Approximation for studying local moment systems, such as Heisenberg and Ising models. Below $T_c$, self-consistency is imposed both for the order parameter and the correlation function. Exact enumeration and Monte-Carlo methods are used to solve the local moment problem on a cluster with coarse-grained effective interactions. Even if the original exchange interactions are short-ranged, the effective interactions are long-ranged. For a single site cluster this method is equivalent to the EDMFT. As the size of the cluster is increased, the fluctuations are systematically included into this approximation. We apply this method to the one-, two- and three-dimensional Ising models. We develop scaling analysis by increasing the cluster size to find the $T_c$. Unlike other expansions about the mean-field theory, our technique converges quite rapidly to the exact solutions, which are known analytically in one and two dimensions and to great accuracy from numerical work in three dimensions. Long-ranged interactions can easily be included in this method, i.e., for studying glassy systems.

11:39AM P11.00003 Performance analysis of continuous-time solvers for quantum impurity models. EMANUELE GULL, Institut fuer theoretische Physik, ETH Zuerich, CH-8093 Zuerich, Switzerland, PHILIPP WERNER, ANDREW MILLIS, Columbia University, 538 West, 120th Street, New York, NY 10027, USA, MATTHIAS TROYER, Institut fuer theoretische Physik, ETH Zuerich, CH-8093 Zuerich, Switzerland — Impurity solvers play an essential role in the numerical investigation of strongly correlated electrons systems within the “dynamical mean field” approximation. Recently, a new class of continuous-time solvers has been developed, based on a diagrammatic expansion of the partition function in either the interactions or the impurity-bath hybridization. We investigate the performance of these two complimentary approaches and compare them to the well-established Hirsch-Fye method. The results show that the continuous-time methods, and in particular the version which expands in the hybridization, provide substantial gains in computational efficiency.

11:51AM P11.00004 Efficient DMFT simulation of the Holstein-Hubbard model. PHILIPP WERNER, ANDREW J. MILLIS, Columbia University — We show that the hybridization expansion algorithm for quantum impurity models [PRl 97, 076405 (2006)] can easily handle a Holstein coupling to phonons. Our approach, which is based on the Lang-Firsov transformation, treats the phonons without approximations and does not affect the overall scaling of the algorithm. We apply the method to the Holstein-Hubbard model in the single site dynamical mean field approximation.

\textsuperscript{1}Support from NSF DMR 0431350

12:03PM P11.00005 Dynamical vertex approximation — a step beyond dynamical mean field theory. ALESSANDRO TOSCHI, Max Planck Institute for Solid State Research, Stuttgart, ANDREY KATANIN, Max Planck Institute for Solid State Research, Stuttgart; Institute of Metal Physics, Ekaterinburg, KARSTEN HELD, Max Planck Institute for Solid State Research, Stuttgart — We have developed a new diagrammatic approach\textsuperscript{[1]}, coined “Dynamical Vertex Approximation” (DFA), with the aim of going beyond dynamical mean field theory for strongly correlated systems, by including the effects of long-range spatial correlations. Without resorting to any finite-size cluster scheme, DFA allows us to compute momentum dependent self-energies (and spectra), whose expressions are diagrammatically constructed starting from the two-particle irreducible local vertex. Therefore, DFA naturally applies for studying effects of magnetic fluctuations with large correlation length in strongly correlated systems, such as the Hubbard model. Specifically, we analyze the interplay between antiferromagnetic fluctuations and the Mott metal-insulator transition in three dimensions and the formation of a pseudogap in two dimensions. The diagrammatic nature of DFA, moreover, should allow for a generalization to the more realistic case of multi-band Hamiltonians. 

\textsuperscript{[1]} A. Toschi, A. Katanin, K. Held, cond-mat/0603100.
12:15PM P11.00006 Optical Spectral Weight of the Hubbard Model – Single-site DMFT Calculation and Comparison to Experimental Data. ARMIN COMANAC, Columbia University, LUCA DE’ MEDI Ci, Rutgers University, MASSIMO CAPONE, Università di Roma La Sapienza, ANDREW J. MILLIS, Columbia University — The single-site dynamical mean field method is used to calculate the variation of optical spectral weight with doping, interaction strength and frequency for the one band Hubbard model. Upper Hubbard band, mid-infrared and coherent quasiparticle contributions are distinguished. It is argued that mid-infrared and coherent contributions can meaningfully be compared to experimental data on transition metal oxide materials such as high-temperature superconductors. The comparison is used to estimate the strength of correlation effects in electron- and hole-doped superconductors.

12:27PM P11.00007 Strong correlations on a triangular lattice: spectral weight suppression on the cobaltates. DIMITRIOS GALANAKIS, Univ. of Illinois at Urbana-Champaign, TUDOR STANESCU, University of Maryland, PHILIP PHILLIPS, Univ. of Illinois at Urbana-Champaign — Two experimental puzzles of strong correlations of the cobaltates (Na$_2$CoO$_2$) are investigated. First the experimental claims that the optical conductivity displays a pseudogap feature. Second the suppression of spectral weight near the chemical potential in the removal spectrum of the x=0.3 material. We address this questions using the 2D Hubbard model in the triangular lattice in the framework of Cluster Dynamical Mean field theory (CDMFT). For x=0.3 we find a suppression of the spectral weight slightly above the chemical potential. The integrated optical conductivity displays no significant transfer of spectral weight from low to high energy as it would be indicative of a pseudogap. Comparison is made with single site, three site and four site clusters.

12:39PM P11.00008 Analysis of the Dynamical Cluster Approximation for the Triangular Lattice Hubbard Model. CHRISTOPHER VARNEY, RICHARD SCAIETTAR, University of California, Davis, MARK JARRELL, ALEXANDRU MACR DIUN, University of Cincinnati, BRIAN MORITZ, University of Waterloo — The behavior of correlated electrons on triangular lattices is attracting increasing interest driven by experimental systems such as the cobaltates. To facilitate understanding of these correlations, we study the Hubbard model using Determinant Quantum Monte Carlo and the Dynamical Cluster Approximation. The spin, charge and pairing response functions obtained with the two methods are compared as a function of spatial lattice and cluster size, respectively, and the one particle spectrum is calculated.

12:51PM P11.00009 NiO - Dynamical Mean Field Study of Charge-Transfer Insulator. J. KUNES, University of Augsburg, Germany, V.I. ANISIMOV, Institute of Metal Physics, Yekaterinburg, Russia, A.V. LUKOYANOV, Ural State Technical University, Yekaterinburg, Russia, D. VOLLHARDT, University of Augsburg, Germany — Charge-transfer (CT) Mott insulators present an important group of transition metal compounds which exhibit phenomena such as metal-insulator transitions or high temperature superconductivity. The location of ligand states between the interaction-split d bands leads to additional complexity, which requires a description beyond a simple Hubbard model. Using a combination of ab initio bandstructure and dynamical mean field theory we study the single particle spectrum of the prototypical CT insulator NiO. Including the O-p orbitals to the Hamiltonian we obtain good agreement with PES and BIS experiments. Notably we find d-peak at the top of the valence band, which cannot be described in static theories, but which is seen in experiment and was reproduced in many-body calculations on small clusters. Studying the effect of doping we find the added holes to occupy the ligand p orbitals despite large Ni-d spectral weight at the valence band. Heavy hole doping leads to a significant reconstruction of the single-particle spectrum and filling of the CT gap. This is the first LDA+DMFT study of charge transfer systems, which includes the p – d hybridization explicitly and is thus able to provide a full description of valence and conduction band spectra.

1:03PM P11.00010 Calculation of Magnetic Exchange Interactions in Mott-Hubbard Systems. QUAN YIN, XIANGANG YIN, SERGEY SAVRASOV, University of California Davis — An efficient method to magnetic exchange interactions in systems with strong electronic correlations is introduced. It is based on a magnetic force theorem which evaluates linear response due to rotations of magnetic moments and uses a novel spectral density functional framework combining our exact diagonalization based LDA+DMFT method. Applications on spin waves and magnetic transition temperatures of 3d transition metal oxides and 5f actinide oxides are in good agreement with experiments.

1:15PM P11.00011 Combined LDA+Exact Diagonalization Study for Actinide Compounds. ALEXEY GORDIENKO, SERGEY SAVRASOV, University of California, Davis — Exact diagonalization (ED) is a most straightforward and powerful way to study problems related to strong electron correlations, but very computationally demanding for f-electron systems. Computational efficiency of the ED approach can be greatly increased with help of iterative methods and we shall present our recent ED implementation which makes use of Kernel Polynomial Method (KPM) to calculate temperature Green’s Function and self-energy. This allows us to deal relatively easy with problems whose size is $5 \times 10^7$ states that is a characteristic for impurity problems with f-electrons. As an application, actinide compounds PuO$_2$ and UO$_2$, will be studied self-consistently using self-energies extracted from cluster ED and combined with electronic structure LDA calculation.

1:27PM P11.00012 Non-collinear magnetism of GdB$_4$: A DFT+$U$ study$.^1$ M. N. HUDA, LEONARD KLEINMAN, Department of Physics, University of Texas at Austin, Texas-78712, USA — Lanthanide-borides show antiferromagnetic behavior where the magnetocrystalline anisotropy plays a major role in their magnetic structures. A recent neutron scattering experiment showed a particular noncollinear behavior of GdB$_4$ at room temperature. We will present our study on the non-collinear magnetism of GdB$_4$ with the GGA + $U$ method with spin orbit coupling. We have found that with or without spin-orbit coupling and with $U$=0 the magnetism is favorably for few meV than the experiment found noncollinear magnetic configuration. Among the noncollinear magnetism configurations that we have studied, when a $U$ parameter and spin-orbit coupling are considered, the experimentally found noncollinear configuration was found to be favorable. However, the value of $U$ parameter is not unique, a range of values were able to get this magnetic order.

$^1$This work was supported by the Welch Foundation (Houston, TX) under grant F-0934.

1:39PM P11.00013 GW+exact diagonalization approach for electronic structure calculations in Mott insulators. NIkolay Zein, RRC “Kurchatov Institute”, Moscow, Serguei Savrasov, UC Davis, CA, Gabriel Kotliar, Rutgers University, NJ — We combine GW and exact diagonalization approaches to calculate electronic structure both in antiferromagnetic and paramagnetic states and find parameters of the corresponding Hubbard model in several transition metal oxides. We discuss extraction of double counting terms, renormalization of one-particle spectrum and interaction, mutual influence of Hubbard-like and GW contributions. Results are compared with LDA+DMFT calculations and the importance of self-consistent approach is stressed.
11:15AM P23.00001 Thin Film Synthesis and Characterization of MAX-Phase Compounds∗†‡, T. H. SCABAROZI, Materials Science and Engineering, Drexel University, W. TAMBUSI, J. D. HETTINGER, S. E. LOFLAND, Department of Physics and Astronomy, Rowan University, M. W. BARSOUM, Materials Science and Engineering, Drexel University — We present the synthesis and characterization of thin film MAX-phase compounds. Thin film synthesis was performed by magnetron sputtering from compound and elemental target materials on 2-inch c-axis sapphire wafers. A series of experiments were carried out where parameters of temperature, gas flow, pressure, and cathode power were varied. Films were characterized by Raman spectroscopy, electron microscopy, X-ray diffraction, and atomic force microscopy. Most films were readily synthesized with multiple-phases which were hexagonal or cubic. All phases were epitaxial, with growth along the (000) and (111) direction for hexagonal and cubic compounds, respectively. With careful control of temperature and stoichiometry, single phase films were produced. Surprisingly, we synthesized Ti$_2$AlC by diffusion of Al from the substrate while only sputtering Ti and C.

†This work was supported by the NSF (DMR-0503711).

11:27AM P23.00002 Composition Dependence of Elastic properties in M$_2$AX Materials∗†‡, T. SCABAROZI, Materials Science and Engineering, Drexel University, S. E. LOFLAND, J. D. HETTINGER, Department of Physics and Astronomy, Rowan University, S. AMINI, P. FINKEL, M. BARSOUM, Materials Science and Engineering, Drexel University — We report on correlations between thermal expansion, elastic moduli, thermal transport, specific heat, and high-temperature x-ray diffractions of materials within the MAX-phase family. Elastic modulus measurements are made using an ultrasonic time of flight technique. Thermal expansion measurements are made using high-temperature x-ray diffractions. We see a clear variation in elastic properties in materials of the form M$_2$AC(M=Ti) with A=S having the largest elastic modulus of all M$_2$AX materials measured to date. It also has the largest Debye temperature as measured from specific heat. The phonon contribution to the thermal conductivity is relatively large, similar in size to the thermal transport resulting from charge carriers. The elastic modulus approaches that found in Ti$_3$SiC$_2$, a M$_3$AX$_2$ material. The overall goal of this work is to correlate measurements of these properties varying M and A to unravel the role of both lattice constituents in determining the elastic properties of this class of materials.

‡This work was supported by NSF DMR-0503711.

11:39AM P23.00003 Structural phase transformations in Ti$_2$Al$_2$Nb system, a first-principles approach∗†‡, MAHDI SANATI, Texas Tech University, DAMIEN WEST, Texas Tech University — First-principles method is employed to determine the vibrational entropy and Gibbs free energy as a function of temperature of the homogenous Ti$_2$Al$_2$Nb system. Calculated energies at T=0 K show instabilities in ternary B2 Ti$_2$Al$_2$Nb alloy against the ω and Ω phases structures. We show that at high temperatures the B2 phase is stabilized by the vibrational entropy. The transition temperatures for B2 → ω and B2 → Ω have been calculated and are in excellent agreement with experiment.

‡This work is supported by the Advanced Research Program of the State of Texas.

11:51AM P23.00004 Precipitation behavior of sigma phase in 304 and 430 stainless steels as hot-rolled at 800°C∗†‡, CHIH-CHUN HSIEH‡, Department of Materials Engineering, National Chung Hsing University, DONG-YIH LIN‡, Department of Materials Science and Engineering, I-Shou University, WEITE WU‡, Department of Materials Engineering, National Chung Hsing University — The effect of various reduction ratios on the precipitation of sigma phase in 304 and 430 stainless steels as hot-rolled at 800°C have been investigated in this study. The sigma phase showed a dendrite-like morphology in the as received materials. A hot rolling process changed the morphology of sigma phase from dendrite-like to globular, especially at higher reduction ratio. The amounts of sigma phase in the stainless steels increased gradually at 800°C with the increasing the reduction ratios from 0 to 75%. The XRD analyses showed that a higher reduction ratio also enhanced the conversion of the delta (110) to sigma (542).

‡The authors are obligated to thank the National Science Council of Taiwan, ROC for its financial support under contracts of NSC93-2216-E-005-002.

12:03PM P11.00015 Kernel sweeping method for exact diagonalization of spin models - numerical computation of a CSL Hamiltonian∗†‡, DARRELL SCHROETER, Occidental College, ELIOT KAPIT, University of Chicago, RONNY THOMALE, MARTIN GREITER, Universität Karlsruhe — We have recently constructed a Hamiltonian that singles out the chiral spin liquid on a square lattice with periodic boundary conditions as the exact and, apart from the two-fold topological degeneracy, unique ground state [1]. The talk will present a kernel-sweeping method that greatly reduces the numerical effort required to perform the exact diagonalization of the Hamiltonian. Results from the calculation of the model on a 4 × 4 lattice, including the spectrum of the model, will be presented. [1] D. F. Schroeter, E. Kapit, R. Thomale, and M. Greiter, Phys. Rev. Lett. in review.

1DS acknowledges support from the Research Corporation under grant CC6682.

12:03PM P23.00005 Intrinsic mechanism of the solid solution softening and hardening in bcc transition metal alloys: combined first principles calculations with atomic row modeling1, N. I. MEDJEDEVA, YU. N. GORNOSTYREV, A. J. FREEMAN, Northwestern U. — The solute–dislocation interaction is of great interest since it determines one of the important strengthening mechanisms in alloys. It is still unclear why some alloying elements lead to hardening but others give rise to softening at low temperature. To reveal the intrinsic mechanisms in solution softening/hardening, the interaction of d transition metal additions with dislocations in bcc metals was studied by using a combined approach including the atomic row model with ab-initio parametrization of interatomic interactions. We found opposite trends in solute-dislocation interaction for the Groups V and VI bcc metals. Additions with extra valence electrons, which enhance the double kink nucleation and result in softening in the Group VI metals, cannot lead to softening in the Group V metals and vice versa: additions with fewer electrons may give rise to softening in the Group V metals but lead to strong hardening in the Group VI metals. We demonstrate that the electronic structure, rather than atomic size or shear modulus misfits, plays an important role in the softening/hardening effects in bcc transition metal alloys.

1AFOSR (Grant No F49620-01-1-0166)

12:15PM P23.00006 Phase field model for recrystallization kinetics, S. SREEKALA, Mechanical and Aerospace Engineering, Princeton University, MIKKO HAATAJA, Mechanical and Aerospace Department, Princeton University — In the recrystallization process, dislocation-free grains grow at the expense of highly deformed matrix. We introduce a phase-field model to study the isothermal recrystallization process as a phase transformation driven by the stored elastic energy which is explicitly non-local due to the long-ranged dislocation strain fields. The dislocations are represented by a coarse-grained Burgers vector density in two spatial dimensions. We have used this model to study the influence of several spatially distinct dislocation distributions (random, cellular and power-law correlated) on the growth kinetics of the recrystallized grain. Our results show that random dislocation distribution produces isotropic growth, whereas the other two distributions show anisotropic and irregular growth as seen in experiments. Also, the growth rate for the random and power-law correlated dislocation distribution follows the JMAK theory rather closely, while the highly anisotropic cell structure shows significant deviations. We demonstrate that the deviations arise from the presence of non-local elastic strain fields.

12:27PM P23.00007 Possible Mechanism of the Pseudogap Formation in Intermetallic Compound Al3V, SUSUMU MIYAHARA, KAZUO TSUMURAYA, Meiji University, JAPAN — The pseudogaps in compounds give a unique electronic character in the materials such as the ones in the skutterudites. The Al3V compound with DO32 structure has also a deep pseudogap that has been explained by the presence of the covalent Al-V and Al-Al bonds in the compound [1]. We propose another possibility of the formation of the pseudogap in the DO32 compound using a density functional method. We introduce a Peierls distortions along c-axis of the double-stacked ordered unit cell, we calculate the density of states and check the gap formation. We will apply the mechanism to the other systems with pseudogap. [1] M. Krajčič and J. Hafner, J. Phys.: Condens. Matter, 14, 1865 (2002).

12:39PM P23.00008 Thermal expansion and magnetostriction in RAi3 (R = Tm,Yb,Lu) single crystals1, S.L. BUD’KO, J. FREDERICA, P.C. CANFIELD, Ames Laboratory and Dept. of Physics and Astronomy, Iowa State University, G.M. SCHMIEDESSHOFF, Dept. of Physics, Occidental College, Los Angeles — We present temperature dependent thermal expansion and low temperature longitudinal magnetostriction measurements taken using a capacitance dilatometer [G.M. Schmiedeshoff et al., RSI, in press] in a PPMS-14 instrument for several cubic RAi3 (R = rare earth) compounds. Quantum oscillations in the magnetostriction were observed in LuAl3 and YbAl3, including few new frequencies for the latter. Data on qualitative changes in the TMAl3 thermal expansion in presence of the longitudinal magnetic field will be presented and discussed.

1This work was supported by DOE, Office of Basic Energy Sciences (SLB, JF, PCC) and NSF (GMS)

12:51PM P23.00009 Theoretical Prediction of Activities in Dilute γ-Ni(Al) Solid Solution at Elevated Temperatures, YONG JIANG, JOHN SMITH, ANTHONY EVANS, UNIVERSITY OF CALIFORNIA, SANTA BARBARA, CA, USA COLLABORATION — For the prediction and interpretation of high-temperature diffusion and related phenomena in multiplayer systems, knowledge of thermodynamic activities is essential. For example, interfacial structures and adhesion strengths of γ-Ni(Al)/Al2O3 at elevated temperatures strongly depend on Al activities. In this study, we present a method for predicting activity coefficients and hence activities in dilute γ-Ni(Al) solid solutions from first-principles. Both thermal lattice vibration and electronic contributions to free energies are considered and compared. Vibrational contributions tend to dominate the temperature dependencies of the free energies: though electron thermal effects are significant. Calculations show opposing temperature trends for the formation enthalpies and entropies, leading to a partial cancellation of their role in the overall energetics. Nevertheless, their remaining temperature effects are strong. Over the temperature range, 400 K < T < 1700 K, the Al activity coefficient varies by 15 orders of magnitude, due to the relative strength of Al-Ni and Al-Al bonds. The Ni activity coefficient only varies less than 4% over the same range. Calculational results compare well with available experimental data. The thermodynamic principles elucidated from the calculations are used to provide a fundamental interpretation.

1:03PM P23.00010 Ab Initio Study of the Effect of Solute Atoms on Stacking Fault Energy in Aluminum, YUE QI, RAJA MISHRA, GM R&D Center — The stacking fault energy (SFE) in binary and ternary alloys of Al with common alloying elements was studied using density functional theory. Among these alloying elements, Fe further increases the SFE and Ge reduces the SFE of Al. The elements increasing the directional inhomogeneity in the electronic charge distribution of the FCC structure correlates with the increasing SFE. The maximum value of charge difference on the fault plane, σmax(Δρ), is used to characterize how much electron has been redistributed due to the stacking fault formation, and the SFE monotonically increases with σmax(Δρ).

1:15PM P23.00011 Thermal stability and diffusion of defects on an Al(100) surface, FRANCESCA BALETTO, NICOLA MARZARI, DMSE-MIT — Understanding and controlling homoepitaxial metal-on-metal growth is a key challenge in surface physics due to its great technological interest. We use a combination of classical and ab-initio techniques, including molecular dynamics and transition-state finding, to identify the dominant mechanisms of diffusion for adatoms and vacancies on an Al(100) surface. We find that exchange and concerted exchange mechanisms, well known in adatom diffusion, play also a central role in vacancy diffusion. In addition, they lead to a distinct phase transition localized in the first layer as temperature is raised.

1:27PM P23.00012 Phonons in nickel and aluminum at elevated temperatures from neutron scattering, MAX KRESCH, OLIVIER DELAIRE, Caltech, REBECCA STEVENS, JIAO LIN, BRENT FULTZ, Caltech — Measurements of the neutron scattering from elemental nickel were made at 10 K, 300 K, 575 K, 875 K and 1275 K, and from elemental aluminum at 10 K, 150 K, 300 K, 525 K and 775 K. From the scattering, the phonon densities-of-states (DOS) were calculated, and subsequently fit to Born von Kármán models of the lattice dynamics. Comparing to previous measurements of thermal expansion, and elastic moduli, we found a small, negative anharmonic contribution to the entropy in both cases. For nickel, we used this to place new bounds on the high temperature magnetic entropy. In both metals, the DOS displayed significant broadening at elevated temperatures. This anharmonic broadening was quantified, and shown to increase approximately as T3.
1:39PM P23.00013 A first principles calculation and statistical mechanics modeling of defects in Al-H system, MIN JI, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory-U.S. DOE. and Department of Physics, Iowa State University, Ames, IA 50011 — The behavior of defects and hydrogen in Al was investigated by first principles calculations and statistical mechanics modeling. The formation energy of different defects in Al-H system such as Al vacancy, H in institution and multiple H in Al vacancy were calculated by first principles method. Defect concentration in thermodynamical equilibrium was studied by total free energy calculation including configuration entropy and defect-defect interaction from low concentration limit to hydride limit. In our grand canonical ensemble model, hydrogen chemical potential under different environment plays an important role in determining the defect concentration and properties in Al-H system.

1:51PM P23.00014 Elastic Constants of Rare Earth and Transition Metal Di-Hydrides¹, C. S. SNOW, J. A. KNAPP, J. F. BROWNING, Sandia National Laboratories — Determinations of the elastic constants of rare earth (RE=Er, La, and) some transition metal (TM=Sc, Ti, Zr) di-hydrides are extremely difficult. Single crystals of these di-hydrides could not be obtained because they break up into fine powders due to the large stresses in the materials caused by the crystallographic changes upon hydriding. However, polycrystalline thin films of these hydrided materials can be grown and are stable over a wide temperature and pressure range. In order to determine the elastic constants of thin metal di-hydride films ab-initio electronic structure calculations using the VASP code have been carried out. These calculations are then compared to bulk and shear moduli measured by a nano-indentation technique. Details and results of the calculations and measurements of the elastic constants of rare earth and transition metal di-hydride films will be presented and a discussion of future applications of this technique will be given.

2:03PM P23.00015 Ab initio electronic and lattice dynamical properties of cerium dihydride, TANJU GUREL, RESUL ERYIGIT, Abant Izzet Baysal University — The rare-earth metal hydrides are interesting systems because of the dramatic structural and electronic changes due to the hydrogen absorption and desorption. Among them, cerium dihydride (CeH₂) is one of the least studied rare-earth metal-hydride.

To have a better understanding, we have performed an ab initio study of electronic and lattice dynamical properties of CeH₂ by using pseudopotential density functional theory within local density approximation (LDA) and a plane-wave basis. Electronic band structure of CeH₂ have been obtained within LDA and as well as GW approximation. Lattice dynamical properties are calculated using density functional perturbation theory. The phonon spectrum is found to contain a set of high-frequency (~ 850-1000 cm⁻¹) optical bands, mostly hydrogen related, and low frequency cerium related acoustic modes climbing to 160 cm⁻¹ at the zone boundary.

Wednesday, March 7, 2007 11:15AM - 1:51PM — Session P31 DCMP: Supersolid Experiments Colorado Convention Center 401

11:15AM P31.00001 Effect of ³He impurity on the supersolid transition of ³He, E. KIM, Korea Advanced Institute of Science and Technology, J. S. XIA, University of Florida, J. T. WEST, X. LIN, M. H. W. CHAN, The Pennsylvania State University — The supersolid phase of ⁴He was reported by a series of torsional oscillator experiments [1]. One of the most striking features of the supersolid transition is the intriguing ³He impurity effect. The addition of an extremely small amount of ³He impurity broadens the transition and enhances the transition temperature Tc. This effect is very different from that in helium film and that in ‘bulk’ superfluid helium. We have studied the influence of ³He impurity on the supersolid transition systematically by progressively diluting isotopically-pure ⁴He (³He impurity less than 2ppb) with ⁴He. The transition temperature is monotonically enhanced with increasing ³He concentration and the supersolid fraction shows a broad maximum around 0.2 ppm. [1] E. Kim and M. H. W. Chan, Science 305, 1941 (2004); Nature 425, 227 (2004); J. Low Temp. Phys. 138, 859 (2005); Phys. Rev. Lett. 97, 115302 (2006).

11:27AM P31.00002 NCRI in Helium Crystals Grown Under Constant Pressure, A.C. CLARK, M.H.W. CHAN, Penn State University — A prominent issue concerning supersolidity in ⁴He is crystal quality. Several theoretical studies have demonstrated that a perfect crystal is insulating. Apparent experimental discrepancies between different laboratories, while very interesting, have not resolved the matter. In the torsional oscillator experiments, all solid samples studied were grown under constant volume. A decrease in pressure occurs during growth so that crystals are forced to expand, possibly resulting in highly strained crystals. There has also been no attempt to seed a single crystal, presumably leading to polycrystallinity. It is known that crystals carefully grown under constant pressure are of high quality. We report on new torsional oscillator measurements of isotopically pure solid ⁴He grown under constant pressure. We detect non-classical rotational inertia (NCRI) in all samples grown to date. Comparisons will be made to earlier studies.

11:39AM P31.00003 Characterization of ⁴He Samples Exhibiting NCRI, M.J. BOWNE, Z. CHENG, J.T. WEST, A.C. CLARK, M.H.W. CHAN, Penn State University — We plan to carry out sound measurements on solid ⁴He samples contained in a torsional oscillator. We believe in situ characterization of samples demonstrating non-classical rotational inertia (NCRI) can lead to a better understanding of the microscopic mechanism behind supersolidity. Sound pulses will be generated and detected with a single quartz transducer housed within the torsion cell. The velocity of sound and attenuation will be extracted from the pulse echoes. This information conveys the relative quality of samples, as well as the orientation of the c-axis for single crystals. Preliminary measurements are under way in a test apparatus.

11:51AM P31.00004 Excess specific heat of solid ⁴He, X. LIN, A. C. CLARK, M. H. W. CHAN, Penn State U. — An experimental challenge on heat capacity measurement is discerning the small specific heat of solid helium from that of the metallic cells typically used to confine the high-pressure solid. We report on heat capacity measurements of solid ⁴He contained in a silicon cell, in our search of a thermodynamic signature of the supersolid phase. Data will be presented for several solid samples around 26 bar, where the heat capacity is at least 10 times larger than that of the silicon cell. Below 200mK we observe a heat capacity in excess of that predicted by Debye theory. It is unclear if our observations are directly associated with the supersolid ⁴He phase. In the hope to elucidate whether this phenomenon is connected to the supersolid phase, we are currently investigating the effect of ³He impurities.
12:03PM P31.00005 Shear measurements of bulk solid $^4$He\(^1\)  
JAMES DAY, JOHN BEAMISH, Department of Physics, University of Alberta — Recent torsional oscillator experiments indicate that the non-classical rotational inertia (NCRI) fraction depends on isotopic purity and on the details of crystal growth and annealing, suggesting that defects may be involved. While solid helium does not flow in response to pressure gradients at low temperatures, plastic deformation of solid helium closer to melting creates defects and pressure gradients which are not easily eliminated by thermal annealing. Similar defects must be created during crystal growth by the blocked capillary method or by large thermal gradients. Given the theoretical arguments against supersolidity in defect-free crystals and the preliminary experimental evidence linking NCRI to annealing, it is important to control and study defects in solid helium more directly. To that effect, we have begun to study the static and low frequency shear deformation of crystals grown by different methods. This is a direct measure of the shear modulus of the crystal and should allow us to separate elastic from inertial effects. We can also compare the elastic to the plastic deformation response by increasing the magnitude of the shear stress applied to the crystal. We will describe our experimental design and present preliminary results.

1This work was supported by NSERC

12:15PM P31.00006 Flow mechanisms of solid $^4$He near melting\(^1\)  
JOHN BEAMISH, JAMES DAY, Department of Physics, University of Alberta — In our recent experiments, we saw no evidence of pressure induced flow of solid helium, neither in the pores of Vycor nor in bulk, in the temperature range where non-classical rotational inertia (NCRI) has been observed; however, we did observed mass flow close to the melting points of our samples. Mass can be transported in crystals through vacancy movement or via the motion of extended defects like dislocations. The high temperature flow of helium confined in Vycor is quite different from that of bulk helium; different mechanisms appear to be involved. In bulk helium the flow is irreversible and is consistent with the creation of defects like dislocations during plastic flow. Plastic flow and dislocation creation cannot occur in nanometer scale channels, and so it is not surprising that we see different behavior for helium in the pores of Vycor. The thermally activated mass flow in Vycor must be due to motion of vacancies or similar point defects. In this talk we will describe the nature of observed flow and possible mechanisms, and discuss its relevance to the NCRI experiments.

1This work was supported by NSERC

12:27PM P31.00007 Effect of Crystal Growth Velocity on “Supersolidity” of $^4$He\(^1\)  
KEIYA SHIRAHAMA, MOTOshi KONDO, SHUNICHI TAKADA, YOSHiyuki SHIBAYAMA, Keio University — One of the most important issues of supersolid studies is to elucidate the relationship between the supersolid behaviors and quality of $^4$He crystal. Recent observation of the annealing effect by Rittner and Reppy suggests that supersolidity is strongly dependent on the sample history. We have examined the effect of crystal growth velocity and crystal annealing on supersolidity of solid $^4$He formed in a cylinder torsional oscillator\(^1\). Solid samples at various pressures are grown by cooling liquid $^4$He under isochoric conditions (blocked capillary method). When the cooling velocity is high (0.1K/min) during crystal growth, the supersolid fraction is 3 times as large as that of slowly grown samples. This supersolid fraction decreased to 1/3 by sample annealings for 1 day near the melting point. On the other hand, no annealing effect is observed in the slowly grown samples. These behaviors strongly suggest that lattice defects formed in the crystal growth process play a crucial role on supersolidity of $^4$He.\(^1\) M.Kondo et al., J.Low.Temp.Phys., to be published

1This work is supported by Grant-in-Aid for Scientific Research on Priority Areas from MEXT, Japan.

12:39PM P31.00008 Influence of sample geometry on the supersolid signal.  
ANN SOPHIE C. RITTNER, JOHN D. REPPY, Cornell University — We have used a torsional oscillator with an annular geometry in order to study the correlation between sample volume and supersolid signals systematically. We varied the width of the annulus in the cell with cylindrical magnesium inserts of different radii. In preliminary measurements on an open cylinder cell, we have found an apparent supersolid fraction $\rho_s$ of 0.04 % at 26 bar, a maximum velocity of 23 $\mu$m/s and a sample volume of 2 cc. In an annular cell with a width of 0.635 mm we measured a supersolid fraction of about 0.33 % at a velocity of 16 $\mu$m/s and a pressure of 32 bar. The increase of the supersolid fraction in restricted geometries suggests that defects cause the NCRI behavior and could explain the different results of previous torsional oscillator measurements.

12:51PM P31.00009 Torsional Oscillator for Studying Supersolid $^4$He at Two Resonant Frequencies\(^1\)  
JOSEPH GRAVES, YUKI AOKI, HARRY KOJIMA, Rutgers University — In order to observe supersolid behavior in solid $^4$He at multiple frequencies while keeping all other parameters constant, an oscillator with two torsional modes has been constructed. The torsion rod is made of beryllium copper and the cylindrical sample chamber is made of Stycast 1266. The two modes have resonant frequencies of 500 and 1200 Hz. Preliminary studies have shown fairly high quality factors of $10^4$ at 300 K and $7 \times 10^4$ at 77 K. We plan to measure the changes, at the two frequencies in the identical solid $^4$He sample, of the resonant frequency, dissipation and critical velocity associated with the supersolid phase at temperatures below 200 mK.

1Supported in part by NSF and by Aresty Research Center for Undergraduates.

1:03PM P31.00010 Search for new evidence of superfluidity in solid $^4$He by phonon propagation\(^1\)  
Yuki Aoki, Harry Kojima, Rutgers University — The phonon propagation generated by heat pulse has been studied in solid $^4$He under pressure between 25 and 56 bar to search for a sign of supersolid behavior at temperatures down to 40 mK. Response to input heat pulses are detected by a titanium film superconducting edge bolometer separated by a 4.5 mm thick solid $^4$He from the heater. According to theoretical studies, a new fourth sound-like mode is expected to emerge in the supersolid state. The sensitivity of our bolometer has been improved from an earlier version by an order of magnitude by changing the film structure for the purpose of searching for a small temperature deviation signal accompanying the fourth sound-like propagation mode. The response of the bolometer to heat pulse was measured in different quality solid samples which had been grown with different cooling rates during solidification. The detected response signal has not revealed any identifiable signature of a new mode within a temperature excursion of about $\Delta T = 5 \mu K$ from the background signal shape. An estimated superflow velocity corresponding to the temperature excursion is greater than the critical velocity observed by Kim and Chan. Our detection sensitivity must be further increased before a definitive conclusion on the fourth sound-like mode can be made.

1Research supported in part by NSF.

1:15PM P31.00011 Debye-Waller factor in solid He-4 at sub-Kelvin temperatures  
ELIZABETH BLACKBURN, JOHN M. GOODKIND, SUNIL K. SINHA, University of California, San Diego, JACOB HUDIS, COLLIN BROHOLM, Johns Hopkins University, JOOST VAN DUIJN, Universidad Complutense de Madrid, Spain, RICHARD DOWN, OLEG KIRICHEK, CHRIS D. FROST, ISIS Facility, Rutherford Appleton Laboratory, UK — The recent observation by Kim and Chan [Science 305 (2204) 1941] of a transition at low temperatures ($\sim 200$ mK) in the hcp-phase of solid helium has re-opened interest in the old question of supersolidity. The nature of the low-temperature phase remains in question, and to investigate this in more detail, we have measured the density distribution of $^4$He nuclei in crystals of $^4$He with a molar volume of 21.3 cm$^3$ down to 140 mK. We find no evidence for any changes in the vicinity of the transition. Treating the material as a traditional crystal, we have extracted the mean square displacement for the nuclei and find anisotropy between the in- and out-of-plane motions. Our values are in agreement with previous work at higher temperatures.
1:27PM P31.00012 Precise neutron diffraction study of hcp and bcc $^{4}$He$^{1}$ — RALPH SIMMONS, ROBERT BLASDELL, Department of Physics, University of Illinois at Urbana-Champaign — Precise lattice parameter measurements are reported for $^{4}$He in both bcc- and hcp phases at low density and low temperature. The results can be used to set limits on a proposed incommensurate equilibrium state of solid $^{4}$He near $T = 0$. "Incommensurate" means a net difference between atomic sites and atoms. The relative difference is defined as $\epsilon$. Present measurements were made by carefully calibrated neutron diffraction. The value established at melting, by comparison with published bulk density values, is $\epsilon = 0.4 \pm 0.4\%$. Much of the uncertainty comes from uncertainties in the bulk values. These neutron results on hcp $^{4}$He are also consistent with previous precise x-ray diffraction work on bcc $^{4}$He and, at higher densities, on both $^{3}$He and $^{4}$He. Published isochoric measurements of changes in x-ray lattice parameters as $T$ is reduced from melting can be used to extrapolate $\epsilon$ toward zero $T$, where its most probable value is zero, with the same uncertainty. The present neutron work on hcp phase agrees with published high-resolution synchrotron x-ray work in showing that the $(c/a)$ ratio is slightly smaller than that corresponding to ideal close-packing.

1Supported in part by DMS under DOE-DE-FG02-91ER45439.

1:39PM P31.00013 New excitations in bcc $^{4}$He — an inelastic neutron scattering study — OSHRI PELLEG, Physics Department, Technion - IIT, Haifa 32000, Israel, JACQUES BOSSY, CNRS, BP 166, 38042 Grenoble Cedex 9, France, MENI SHAY, SLAVA SORKIN, EMIL POLTURAK, Physics Department, Technion - IIT, Haifa 32000, Israel — We report results of inelastic neutron scattering experiments on bcc solid $^{4}$He (Pelleg et al. Phys. Rev. B. 73, 180301(R) (2006)). In the experiments, we studied the excitation spectrum of the solid, including the phonon branches and the recently discovered "optic-like" branch (T. Markovich et al., Phys. Rev. Lett. 88, 195301(2002)). We were able to determine that the new "optic-like" branch has an intrinsic dispersion, hence it is a propagating mode. This excitation also couples to the usual phonons. In addition, in the new experiments we discovered another "optic-like" branch. The second "optic-like" branch is dispersionless, with an energy around 1 meV ($\sim$ 11K). This excitation does not seem to couple to phonons. Hence, the properties of the two "optic-like" branches seem different. Since one expects only 3 acoustic phonon branches in a monoatomic cubic crystal, these two new branches must represent some different type of excitations. Some potential interpretations, based on Path Integral Monte Carlo simulations, will be presented.

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Wednesday, March 7, 2007 2:30PM - 5:30PM — Session S1 DCMP: Magnetic Excitations in High Tc Superconductors Colorado Convention Center Four Seasons A-B

2:30PM S1.00001 Spin Dynamics in the electron-doped high-$T_c$ superconductors Pr$_{0.88}$LaCe$_{0.12}$CuO$_{4-\delta}^{6+}$ — PENGCHENG DAI, The University of Tennessee — We briefly review results of recent neutron scattering experiments designed to probe the evolution of antiferromagnetic (AF) order and spin dynamics in the electron- doped Pr$_{0.88}$LaCe$_{0.12}$CuO$_{4-\delta}$ (PLCCO) as the system is tuned from its as-grown non-superconducting AF state into an optimally doped superconductor ($T_c = 27.5$ K) without static AF order [1-3]. For under doped materials, a quasi-two- dimensional spin-density wave was found to coexist with three- dimensional AF order and superconductivity. In addition, the low-energy spin excitations follow Bose statistics. In the case of optimally doped material, we have discovered a magnetic resonance intimately related to superconductivity analogous to the resonance in hole-doped materials. On the other hand, the low energy spin excitations have very weak temperature dependence and do not follow Bose statistics, in sharp contrast to the as-grown nonsuperconducting materials. 1 Stephen D. Wilson, Pengcheng Dai, Shiliang Li, Songxue Chi, H. J. Kang, and J. W. Lynn, Nature (London) 442, 59 (2006). 2 Stephen D. Wilson, Shiliang Li, Hyungyeo Woo, Pengcheng Dai, H. A. Mook, C. D. Frost, S. Komiya, and Y. Ando, Phys. Rev. Lett. 96, 157001 (2006). 3 Stephen D. Wilson, Shiliang Li, Pengcheng Dai, Wei Bao, J. H. Chung, H. J. Kang, S.-H. Lee, S. Komiya, and Y. Ando, Phys. Rev. B 74, 144514 (2006).

3:06PM S1.00002 Spin dynamics of YBa$_2$Cu$_3$O$_{6+\delta}$ — BERNHARD KEIMER, Max-Planck-Institute for Solid State Research — We have used inelastically scattered neutrons to determine the spin dynamics in unwinned single crystals of YBa$_2$Cu$_3$O$_{6+\delta}$, over a wide range of doping levels [1], with particular attention on its in-plane anisotropy [2]. Among other observations, we have found that the spin dynamics in the superconducting and pseudogap states are qualitatively different. The results allow incisive tests of current theories; including in particular theories based on static and fluctuating spin-charge stripes. We will also present initial results of an effort to provide a quantitative description of both the spin dynamics and the charge dynamics (determined by infrared and angle-resolved photoemission spectroscopies [3]) in the same YBa$_2$Cu$_3$O$_{6+\delta}$ single crystals. [1] S. Pailhes et al., Phys. Rev. Lett. 93, 167001 (2004); Phys. Rev. Lett. 96, 257001 (2006). [2] V. Hinkov et al., Nature 430, 650 (2004); cond-mat/0601048. [3] V. S. Borisenko et al., Phys. Rev. Lett. 96, 117004 (2006); V. B. Zabolotnyy et al., cond-mat/0608295.

3:42PM S1.00003 New Insight into an Under-doped Regime of High Tc Superconductivity - NMR Studies of Multi-layered Cuprates — YOSHIKO KITAOKA, Osaka University — High-temperature superconductivity (HTSC) has not been fully understood yet despite 20 year’s intensive research. In particular, a possible interplay between antiferromagnetism (AFM) and HTSC remains as a most interesting problem. It is believed that they all fit into a universal phase diagram which suggests a competition between AFM and HTSC. Recently, however, through the systematic NMR experiments on the Ho, Ti- and Cu-based five-layered HTSC, we propose a novel phase diagram [1-3], which differs from the generic phase diagram of the HTSC reported so far, for instance, such as LSCO. The five-layered HTSC compounds include two types of CuO$_2$ planes, an outer CuO$_2$ plane (OP) in a pyramidal coordination and an inner CuO$_2$ plane (IP) in a square one with no apical oxygen. Remarkable feature of the multi-layered HTSC is the presence of ideally flat CuO$_2$ planes that are homogeneously doped, which is ensured by the narrowest NMR spectral width among the various Ho and Ti-based HTSC. It should be noted that the nearly non-doped AFM in the IP and the IP* phase takes place, whereas inhomogeneous magnetic phases such as spin-glass phase or stripe phase are not observed at both the IP’s and the OP’s. Instead, the existence of the doped AFM metallic (AFMM) phase at the IP and the IP* is remarkable at the boundary between AFM insulating (AFMI) phase and SC. This differs from the case of LSCO where the disorder-driven magnetic phases exist between the AFMI phase in $N_d < 0.02$ and the SC phase in $N_d > 0.05$. In an underlying phase diagram, the AFMM is extended to a higher hole density due to the flatness of CuO$_2$ plane without any apical oxygen and homogeneous distribution of carrier density. By contrast, the coexistence phase diagrams reported thus far under the inevitable disorder effect associated with the chemical substitution introduced into the CuO$_2$ out-of-planes as corroborated by the observation of a disorder-driven transition between AFMM phase to AFMI phase found in the Cu-based multi-layered system [3]. Through the discovery of the uniform mixing of AFM and HTSC in a single CuO$_2$ layer (OP) at Hg-1245(UD) with $M_{AFM} = 0.15\%$ and $T_c = 72$ K, we will shed new light on the generic phase diagram of HTSC in the under-doped regimes. Namely, both phases may be mediated by the same magnetic interaction. It is this global phase diagram presented here to make one convince the presence of the AFM+SC uniformly coexisting phase. From the results presented in this talk, we may also raise a question: Do we need a bosonic glue to pair electrons in the uniformly coexisting state of AFM and SC? References: [1] H. Mukuda et al. Phys. Rev. Lett. 96, 087001 (2006); [2] N. Shimizu et al., submitted to PRL (2006). [3] H. Mukuda et al., J. Phys. Soc. Jpn. 75, No.12 (2006).

3These works have been done in collaboration with H. Mukuda, M. Abe, S Shimizu.
4:20PM S1.00004 Two Energy Scales in the Spin Excitations of La$_2$-$_x$Sr$_x$CuO$_4$. STEPHEN HAYDEN, University of Bristol — There has recently been considerable progress in electronic quasiparticle spectroscopy of high-$T_c$ superconductors. Angle resolved photoemission and tunnelling indicate that the quasiparticles are strongly coupled to excitations with energies in the range 40-70 meV. The recent debate has focused around phonons being the coupled excitations. The focus on phonons is largely because high-resolution phonon spectra are available and they contain considerable structure. Collective spin excitations are promising candidates for the strongly coupled excitations. However high resolution neutron data in the relevant 40-70 meV energy range have not been available for compounds where the quasiparticle anomalies are observed. In order to fill this gap in our knowledge, we have prepared 50g of single crystals of La$_{1.84}$Sr$_{0.16}$CuO$_4$ and carried out a new study of the magnetic excitations over a wide energy range, with considerably better energy resolution than our previous studies, and with good momentum resolution. Experiments were carried out using the MAPS spectrometer at the ISIS spallation neutron source. Our results demonstrate that the magnetic excitations have a two component structure with a low-frequency component strongest around 18 meV and a broader component strongest near 40-70 meV. The second component carries most of the spectral weight and its energy matches structure seen in photoemission and tunnelling spectra in the range 50-90 meV. Thus collective spin excitations may explain features of quasiparticle spectroscopies and are therefore likely to be strongly coupled excitations. The high-frequency excitations are most naturally interpreted as being due to residual antiferromagnetic interactions.

leading to a destructive regime predicted by de Gennes. Extending our previous work that confirmed de Gennes’ prediction, we have discovered the existence of a flux-dependent superfluid velocity, determined by fluxoid quantization, becomes comparable to or higher than the superconducting condensation energy.

1. Upon lowering the temperature, larger changes in \( \xi \) occur. Below approximately 0.3 \( T_c \), the final state after a transition is close to the ground state. The dynamics leading to this phenomenon are discussed in terms of the time dependent Ginzburg-Landau theory for gapless and gapped superconductors and a qualitative explanation based on the formation of a local hot spot.

2. Work supported by AFOSR and NSF.

3. Work supported by NSF.

4:18PM S3.00004 Aharonov-Bohm effect in the spin-incoherent regime of strongly correlated 1D electrons , MARKUS KINDERMANN, Georgia Institute of Technology — Recently the spin-incoherent regime of the interacting one-dimensional electron gas has received much attention. In this regime the exchange coupling of nearest neighbor spins is so small that it is completely disrupted by the thermal motion. This regime is generic to low density 1D systems. It is not captured by the standard Luttinger liquid theory and it is expected to exhibit a number of anomalous properties. One of its unusual features is an anomalous conductance suppression reminiscent of conductance reductions observed in quantum wires and point contacts. Despite its great theoretical interest spin incoherence has not yet been demonstrated conclusively in experiments and specific probes of the regime are needed. In this talk I will discuss various tunneling and Aharonov-Bohm interferference geometries [1] that can serve this purpose. Spin incoherence will be shown to have a number of distinctive signatures in such experiments such as magnetic field dependent tunneling exponents [2], a strong magnetic field dependence of the interference contrast, and an anomalous scaling of this contrast with the applied voltage [1]. In collaboration with P.W. Brouwer and A.J. Millis. [1] M. Kindermann, P. W. Brouwer, and A. J. Millis, Phys. Rev. Lett. 97, 036809 (2006). [2] M. Kindermann and P. W. Brouwer, Phys. Rev. B 74, 115121 (2006).
3:42PM S8.00007 Microscopic theory of thermal phase slips in clean narrow superconducting wires\textsuperscript{1}. ALEXANDER ZHAROV, ANDREI LOPATIN, ALEXEI KOSHELEV, VALERII VINOKUR, Argonne National Laboratory — We consider structure of a thermal phase slip center for a simple microscopic model of a clean one-dimensional superconductors in which superconductivity occurs only within one conducting channel or several identical channels. Surprisingly, the Eilenberger equations describing the saddle-point configuration allow for exact analytical solution in the whole temperature and current range. This solution allows us to derive a closed expression for the free-energy barrier, which we use to compute its temperature and current dependences.

\textsuperscript{1}This work was supported by the U. S. DOE, Office of Science, under contract # DE-AC02-06CH11357.

3:54PM S8.00008 Vortices in superconducting nanoshells. JACQUES TEMPERE, VLADIMIR GLADILIN, Universiteit Antwerpen, ISAAC SILVERA, Harvard University, JOZEF DEVREESE, Universiteit Antwerpen — A nanoshell consists of a nanoscopic grain of insulator (typically SiO\textsubscript{2}) on which a thin layer of metal is deposited. If the material used to make the thin shell is superconducting, the nanoshell itself will exhibit superconducting order. When the superconducting nanoshell is placed in a magnetic field, vortices can be nucleated near the equator of the spherical shell, and will move towards the poles of the nanoshell where they are trapped. Using the Ginzburg-Landau equations adapted for the spherical geometry, we investigate the possibility for giant vorticity and multi-vortex states on thin spherical shells, as a function of shell radius and magnetic field. Furthermore we show that this nanostructure shows potential for flux trapping, as it has a strong magnetization hysteresis.

4:06PM S8.00009 Proximity induced superconductivity and multiple Andreev reflections in Graphene, ALEXANDROS SHAILOS, WILLY NATIVEL, ALIK KASUMOV, CHRISTIAN COLLET, MEYDI FERRIER, SOPHIE GUÉRON, RICHARD DEBLOCK, HÉLÈNE BOUCHIAT, LPS MESOSCOPIC TEAM, THALES TEAM — We have investigated electronic transport of a graphene layer connected to superconducting electrodes. The device is prepared by mechanical exfoliation of graphite. A small mesa of graphene is placed on top of a silicon substrate covered by Alumina and 2 electrodes of tungsten separated by 2.5 microns are grown using a focus ion beam. Whereas tungsten electrodes are superconducting below 4K, proximity induced superconductivity in graphene is observed below 1K with a large differential resistance drop at low bias voltage. Signatures of multiple Andreev reflections are observed as peaks located at voltages corresponding to sub-multiple values of 2e\textDelta. The scale of the graphene electrodes.

4:18PM S8.00010 Size quantization effect in graphite based proximity systems, ANDREAS BILL, California State University Long Beach, 1250 Bellflower Blvd., Long Beach, CA 90840, VLADIMIR Z. KRESIN, Lawrence Berkeley National Laboratory, University of California at Berkeley, Berkeley, CA 94720 — We discuss size-quantization (SQ) effects in a proximity system made of a graphite thin film deposited onto a superconductor. We show that SQ leads to oscillations of the superconducting critical temperature \(T_c\) as a function of the thickness of the graphite layer. This oscillation is due to the peculiar behavior of the density of states in size-quantized systems. The calculated period is directly related to major parameters of the semimetal and thus to the normal state properties of the bilayer. Recent experiments made on graphite/superconductor bilayers are discussed in the framework of the theory.

4:30PM S8.00011 Theory of superconductivity in multiwall carbon nanotubes, ENRICO PERFETTO, CNISM, Universita’ di Roma Tor Vergata (Italy), JOSE GONZALEZ, CSIC-Madrid (Spain) — Recently superconductivity has been observed at 12K in multiwall carbon nanotubes (MWNts). The key feature in the experimental setup is that almost all the shells in the MWNts are electrically active. Here we propose a model for the MWNts where the electrons live in a large number of coupled one-dimensional systems, reminiscent of the hexagonal Fermi surface of the MWNts. We pay attention to the competition between the screened Coulomb repulsion and phonon-mediated electron-electron interaction. The low-energy behaviour of the model is studied with one-loop renormalization group. We find that by lowering the energy scale the inter-shell Cooper pair tunnelling amplitude grows up, inducing a superconducting instability with p-wave order parameter. The phase diagram shows that the superconducting phase dominates for large radii of the MWNts and by doping the system. At low doping and small radius a competition with charge density wave instability is observed.

4:42PM S8.00012 Synthesis and characterization of superconducting NbN nanowires and nanoribbons, U. PATEL*, Z. L. XIAO*, H. CLAUS, J. HUA*, R. DIVAN, U. WELP, W. K. KWOK, Argonne National Laboratory; *also at Northern Illinois University — The role of one-dimensional nanostructures has recently gained wide importance due to their novel properties and potential applications in electronics. Here, we report a two-step approach to synthesize one-dimensional superconducting NbN nanowires and nanoribbons by converting NbSe\textsubscript{3} nanostuctures. First, NbSe\textsubscript{3} nanostucture precursors were prepared by sintering niobium and selenium powders in a evacuated quartz tube. Subsequently, these NbSe\textsubscript{3} nanostuctures were transformed into NbN under an atmosphere of ammonia gas at a reaction temperature of up to 1000 °C. Superconducting transition temperatures up to 10 K were obtained from both magnetization and four-probe transport measurements. We also carried out morphology and structural characterizations of these NbN nanostructures. This material is based upon work supported by the US Department of Energy, under Award Numbers DE-FG02-06ER46334 and DE-AC02-06CH11357.

5:06PM S8.00013 Magnetoresistance of granular superconductors at low temperatures, IGOR BELOBORODOV, Argonne National Laboratory — I will discuss the resistivity of granular superconductors in the presence of magnetic field at low temperatures. It is assumed that the tunneling between grains is large such that all conventional effects of localization can be neglected. I will show that at low temperatures the superconducting fluctuations reduce the one-particle density of states but do not contribute to transport. As a result the resistivity in the transition region exceeds the normal state value leading to a negative magnetoresistance. I will also analyze the possibility of the formation of a magnetic field induced insulating state in a two dimensional granular superconductors and show that such a state appears in a model with spatial variations of the single grain critical magnetic field. This model describes realistic granular samples with the dispersion in grain sizes and explains a mechanism leading to a giant peak in the magnetoresistance.

5:45PM S8.00014 Interplay between electronic transport and mechanical degrees of freedom in metallic atomic-size contacts, ALEKSEI MARCHENKOV, ZHENTING DAI, BRANDON DONEHOO, CHUN ZHANG, ROBERT BARNETT, UZI LANDMAN, Georgia Institute of Technology — Comprehensive measurements of transport properties of the smallest metallic contacts, both in normal and superconducting states, may provide sufficient information to identify their atomic structure. We demonstrated completely reversible mechanical manipulation of the electronic state of niobium atomic-size contacts. This regime includes switching between two distinct configurations manifested as two-level conductance fluctuations. Synergetic first-principles numerical modeling of the structure and transport properties, based on the combination of the Density Functional Theory and Non-Equilibrium Green’s Functions formalism, revealed that these contacts consist of niobium dimers trapped between apexes of bulk leads. The observed bistability was associated with the dimer shuttling between a symmetric and an asymmetric configurations in the gap. Point contact spectroscopy of these configurations reveals, on top of the expected signatures due to phonon modes, features, which we associate with the excitation of the vibrational modes of the trapped dimer. Finally, we discuss the evidence that these vibrations can be caused by the intrinsic Josephson radiation.
2:30PM S23.00001 Quantum Monte Carlo determination of the equation of state of cubic boron nitride, K.P. ESLER, B. MILITZER, R.E. COHEN, Carnegie Institution of Washington — The pressure inside a diamond anvil cell is usually determined by measuring the pressure-dependent frequency shift of a small ruby sample or by x-ray diffraction on a small chip of a pressure standard. However, there are no primary pressure standards for the megabar range. Recently, cubic boron nitride (cBN) has been suggested as an accurate pressure gauge. Unlike ruby, its structure is highly constrained by symmetry and stable beyond 100 GPa, and it has a well-separated Raman spectrum with sufficient pressure dependence to allow accurate pressure calibration. Its use as a pressure standard requires reliable equation of state (EOS) data. A density functional theory (DFT) calculation of the cBN EOS based on the generalized gradient approximation agrees well with experiment up to 100 GPa, but a calculation that does not depend on an approximate exchange-correlation functional would be desirable. Quantum Monte Carlo (QMC) is a correlated, first-principles simulation method with fewer uncontrolled approximations than DFT methods. We present the results of applying state-of-the-art QMC methods to the bulk cBN solid in order to determine the EOS. ① A.F. Goncharov et al., Phys. Rev. B 72, 100104R (2005).

2:42PM S23.00002 First-principles study of cubic BC6N: Structural forms and ideal strength, YI ZHANG, Department of Physics, University of Nevada, Las Vegas, HONG SUN, Department of Physics, Shanghai Jiao Tong University, China, CHANGFENG CHEN, Department of Physics, University of Nevada, Las Vegas — We present first-principles calculations on the structural forms and ideal strength of cubic BC6N. The calculated ideal tensile and shear strength are lower or comparable to those of c-BN. Our results show that increasing carbon content does not lead to significant enhancement of the ideal strength as expected by the conventional wisdom. It can be attributed to the weak C-N bonds that impose a limit on the idea strength.

2:54PM S23.00003 Towards a multiphase equation of state of Carbon from first principles, ALFREDO CORREA, University of California at Berkeley and Lawrence Livermore National Laboratory, LORIN BENEDICT, ERIC SCHWEGLER, Lawrence Livermore National Laboratory — Ab initio molecular dynamics and electronic structure calculation had become one of the most useful tools to investigate properties of materials. Unfortunately these atomistic detailed results are rarely reused in calculations at a higher level of description, such as fluid dynamics and finite elements calculations. In this talk we present a concrete example showing the way that first principles results can be expressed in a way that is useful for hydrodynamics calculations, in particular we show how to build an analytic equation of state for Carbon that involves solid (diamond and BC8) and liquid phases. Applications of this newly obtained equation of state will be presented. This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

3:06PM S23.00004 VLab: A Collaborative Grid/Portal System for Computations of Materials Properties at High Pressures and Temperatures, PEDRO DA SILVEIRA, Minnesota Supercomputing Institute, University of Minnesota. CESAR R. S. DA SILVA, Minnesota Supercomputing Institute, University of Minnesota, RENATA M. WENTZCOVITCH, Minnesota Supercomputing Institute, University of Minnesota — We describe the development of a collaborative service-oriented architecture, the VLab, which handles from a single workflow the concurrent and distributed execution of multiple tasks involved in complex sequences of first principles calculations of materials properties at high pressures and temperatures. We demonstrate the usefulness of this system through a consolidated portal interface.

3:18PM S23.00005 Shock-wave propagation in carbon nanotube reinforced a-SiC composites, DEEPAK SRIVASTAVA, MAXIM MAKEEV, NASA Ames Research Center, MS 229-1, Moffett Field, CA 94035 — We have performed state-of-the-art large-scale molecular dynamics simulation study of shock-wave propagation in amorphous silicon carbide (a-SiC) and carbon nanotube (CNT) reinforced a-SiC composites. The materials response, shock-wave structure, damage evolution and properties in shock-loaded CNT/a-SiC composites are found to differ significantly from the similar shock wave propagation in pristine a-SiC sample. The effects of CNTs on the shock-wave velocity and profile are investigated and analyzed in detail. In all the considered cases, a significant densification is observed in the shock-loaded regions. In the case of CNTs aligned perpendicular to the impact direction, the shock-wave causes CNTs to collapse, while in the case of CNTs oriented parallel to the impact direction the structure of the CNTs is preserved and a channeling of the resulting compressive wave is observed which leads to material sputtering at the bottom surface. The micro-structural changes in the after shock region will be discussed in this presentation.

3:30PM S23.00006 Molecular Dynamics Simulations of Hypervelocity Impacts, ELI T. OWENS, MARTINA E. BACHLECHNER, Physics Department, West Virginia University — Outer space silicon solar cells are exposed to impacts with micro meteors that can destroy the surface leading to device failure. A protective coating of silicon nitride will protect against such failure. Large-scale molecular dynamics simulations are used to study how silicon/silicon nitride fails due to hypervelocity impacts. Three impactors made of silicon nitride are studied. Their cross-sectional areas, relative to the target, are as follows: the same as the target, half of the target, and a quarter of the target. Impactor speeds from 5 to 11 km/sec. The structural modes of failure, such as deformation of the target by the impactor and delamination of the silicon nitride from the silicon at the interface. These simulations will give a much clearer picture of how silicon cells composed of a silicon/silicon nitride interface will respond to impacts in outer space. This will ultimately lead to improved devices with longer life spans.

① Research supported by NSF/EAR and NSF/ITR programs.

② Work is supported by the NASA West Virginia Space Grant Consortium as well as a Barry M. Goldwater Scholarship.
3:42PM S23.00007 The generation of dissipative structures in solids at high pressures. ROGER W. MINICH, Lawrence Livermore National Laboratory, DANIEL ORLIKOWSKI, JEFF H. NGUYEN — The recent ability to tailor pressure drives up to and exceeding a Mbar has led to the ability to study the response of materials along different thermodynamic paths that may be significantly different from a Hugoniot. Observations of recent data suggest that a ramped pressure drive generates coherent structures that behave like solitons in the weakly dissipative limit, but later form kinks which localize the dissipation and coalesce into ever increasing larger kinks in time. The experimental observations are discussed in the context of the KdV-Burgers equation and a universal scaling law is proposed in the limit of high dissipation. This work was performed under the auspices of the U.S. Department of Energy by the California Livermore National Laboratory under contract W-7405-Eng-48.

3:54PM S23.00008 Large scale MD Simulations of the time-resolved optical properties of warm dense metals. S. MAZEVET, J. CLEROUNIN, L. SOULARD, Département de Physique Théorique et Appliquée, CEA/DAM Ile-de-France/BP12, 91680 Bruyères-le-Châtel Cedex, France — Recent experiments on gold suggest that the electrical and optical properties of metals in the warm dense matter regime can be accessed by performing time-resolved measurements after the illumination of a metallic thin film by a short-pulse laser[1]. The non-equilibrium situation created in this experimental setup poses new challenges to simulation methods as the time evolution of the atomic structure needs to be followed as the metal evolves from a solid to a plasma state. We used a combination of ab-initio and large scale molecular dynamics simulations to calculate the evolution of the atomic structure, and the electrical conductivity of various metals during the first pico-seconds after a short-pulse laser illumination.

4:06PM S23.00009 Dynamics of ultracold neutral plasma1. LEE COLLINS, T-04, Los Alamos National Laboratory, BYOUNGSEON JEON, Dept. Applied Science, UC.Davis/T-12, Los Alamos National Laboratory, JOEL KRESS, T-12, Los Alamos National Laboratory, NIELS GRONBECH-JENSEN, Dept. Applied Science, UC.Davis — For an ultracold neutral plasma produced by photoionization of laser-cooled heavy particles, initial expansion behavior was studied with classical molecular dynamics. To investigate huge particle sets under open boundary condition, the TREE method has been implemented and Rydberg states of low quantum number were studied. We also examined the degree of ion correlation.

4:18PM S23.00010 Hot and Cold Ionization of Strongly Coupled Plasmas Generated by Intense Shock Waves, VLADIMIR FORTOV, Institute for High Energy Density of RAS — The physical properties of strongly coupled plasmas at high pressures and energy densities are analyzed in a broad region of parameters. The theoretical and experimental methods of non-ideal plasma investigations are discussed. Main attention is paid to the dynamical methods. Intense shock, rarefaction, and radiative waves in solid and porous samples, and electrical explosion were used for generation of high density plasmas at extremely high pressure. The pressure ionization plasma phenomena in hydrogen, helium, noble gases, iodine, silica, sulfur, H2O, fullerenes and some metals are analyzed on the base of multiple shock wave experiments. The data obtained were described by the non-ideal plasma model taking into account increase of charge carrier number as a result of “temperature” and “pressure” ionization. In contrast to these experiments the multiple shock compression of solid Li, Ca and Na shows strong modification of electron plasma energy spectrum and as a result of that - dielectricization of these elements at megabars. The “plasma” phase transition phenomena are analyzed on the base of shock experiments and quantum Monte-Carlo simulations.

4:30PM S23.00011 Relaxation of laser-induced two component plasma1. BYOUNGSEON JEON, Dept. Applied Science, UC.Davis/T-12, Los Alamos National Laboratory, LEE COLLINS, T-04, Los Alamos National Laboratory, JOEL KRESS, T-12, Los Alamos National Laboratory, NIELS GRONBECH-JENSEN, Dept. Applied Science, UC.Davis — In inertial-confined fusion plasmas, the ions and electrons can exist in a non-equilibrium state. Using classical molecular dynamics, we have studied a two-temperature plasma under extreme conditions and determined system properties. The temperature relaxation rate and diffusion coefficients of each species were found, and the results were compared with the Spitzer and other relaxation formulæ.

4:42PM S23.00012 First Principles Molecular Dynamics Simulations of Diopside Liquid at High Pressure, NI SUN, LARS STIXRUDE, University of Michigan, BIJAYA KARKI, Louisiana State University — Diopside (CaMgSi2O6) is a major component of basalt; the high-pressure end members, Mg-perovskite (MgSiO3) and Ca-perovskite (CaSiO3), make up more than 80 % of the lower mantle. Despite its importance, most studies of diopside liquid have been performed at relatively low pressures and temperatures. In this study, we investigated CaMgSi2O6 liquid at lower mantle conditions by first principles molecular dynamics (FPMD) simulations based on density functional theory. The average Si-O coordination number increases nearly linearly from 4 to 6 with two-fold compression. The structure shows evidence of incipient exsolution with non-random clustering of Mg and Ca ions. Our results are well fitted by Mie-Grüneisen equation of state with a Grüneisen parameter that increases on compression. The variation of the diffusion coefficient with pressure and temperature is captured by the Arrhenius relation with activation energy and volume E* = 1.2 eV and V* = 1.25 A3. The electronic properties of CaMgSi2O6 liquid phase are similar as those of the MgSiO3 liquid: there is no band gap and an extra peak appears at the Fermi level at low pressure.

Wednesday, March 7, 2007 2:30PM - 5:18PM – Session S31 DCMP: Quantum Fluids Colorado Convention Center 401

2:30PM S31.00001 High Frequency Transverse Acoustics in Superfluid 3He. JOHN P. DAVIS, HYOUNG-SONO CHOI, JOHANNES POLLANEN, WILLIAM P. HALPERIN, Northwestern University — Acoustic studies of superfluid 3He have a rich history and have contributed significantly to our understanding. Recently we have made technical advances that have allowed us to extend transverse acoustic measurements to much higher frequencies. We will discuss these techniques, as they are applicable to a broad range of acoustic measurements. The relevant frequency in superfluid 3He is associated with the pair energy, which varies from 69 to 194 MHz in the range of 0 to 34 bar. With our improved acoustic response, up to the 200 MHz range, we can probe the structure of the order parameter deep into the superfluid at higher pressures than before. This has allowed us to make precision measurements of one of the collective modes of superfluid 3He, the Imaginary Squashing Mode [1]. From these measurements we have extracted values for the strength of f-wave pairing interactions in this dominantly p-wave superfluid. We will discuss our results in comparison with earlier measurements from the Acoustic Faraday Effect [2]. [1] J.P. Davis, H.Choi, J. Pollanen, and W.P. Halperin, Phys. Rev. Lett. 97, 115301 (2006). [2] Y. Lee, T.M. Haard, W.P. Halperin and J.A. Sauls, Nature 400, 431 (1999).
The energy dissipation of the vortex moving through the mesh can exceed the loss rate from mutual friction by 50% to 100%.

An artificially high friction coefficient. We find that as the vortex moves, reconnections with pinned vortices can reduce its length, and hence its line energy.

Move at the local superfluid velocity, and by allowing for reconnections when two vortices approach closely. To keep the simulation run time practical, we use to the cell wall and annihilate, leaving behind fragments pinned at any microscopic wall roughness. We simulate the situation by requiring the free vortex to overcome thermally, and pinning at a flat end is the hardest. This pattern would not be expected from considerations of vortex line energy alone. We take no external disturbance, it remains indefinitely. We briefly heat the cell and find the temperature at which the vortex depins. By observing the vortex motion at each end at either a rounded bump, a conical indentation, or a flat surface. With the cryostat stationary, we measure the persistence of the vortex. With

Warren, R.J. Zieve, UC Davis — We have observed experimentally that a vortex moving in a cylindrical cell loses energy up to eight orders of magnitude more than expected from bulk mutual friction alone. Here we investigate the possibility that reconnections with a mesh of small vortices pinned to the cell wall dominate the energy loss. Such pinned vortices may be an unavoidable consequence of rotating the cylinder. Once rotation ceases, most vortices move to the cell wall and annihilate, leaving behind fragments pinned at any microscopic wall roughness. We simulate the situation by requiring the free vortex to move at the local superfluid velocity, and by allowing for reconnections when two vortices approach closely. To keep the simulation run time practical, we use an artificially high friction coefficient. We find that as the vortex moves, reconnections with pinned vortices can reduce its length, and hence its line energy. The energy dissipation of the vortex moving through the mesh can exceed the loss rate from mutual friction by 50% to 100%.

The energy gap at North and South Poles of the Fermi sphere and is anisotropic. A unit vector directing from the South Pole to the North Pole is referred to as the $\ell$ vector. The $\ell$ vector tends to align parallel to a surface normal. The conductivity of the Wigner solid is sensitive to the quasiparticle distribution, and hence, sensitive to the alignment of the $\ell$ vector. Our observation is in good agreement with the abovementioned picture of the $\ell$ vector alignment. In the B-phase the situation is more subtle. Nevertheless, our observation gives a strong support for the present understanding of the magnetic-field-induced anisotropy of the B-phase.

Understanding Superfluid $^3$He by Determining $\beta$-Coefficients of Ginzburg-Landau Theory, H. Choi, J.P. Davis, J. Pollanen, W.P. Halperin, Northwestern University, Evanston, IL 60208, USA — The Ginzburg-Landau (GL) theory is a phenomenological theory that is used to characterize thermodynamic properties of a system near a phase transition. The free energy is expressed as an expansion of the order parameter and for superfluid $^3$He there is one second order term and five fourth order terms. Since the GL theory is a phenomenological theory, one can determine the coefficients to these terms empirically; however, existing experiments are unable to determine all five fourth order coefficients, the $\beta$'s. To date, only four different combinations of $\beta$'s are known [1]. In the case of superfluid $^3$He, using quasiclassical theory, the coefficients have been calculated [2]. We used the calculation as a guide to construct a model to define all five $\beta$'s independently. The model provides us with the full understanding of the GL theory for $^3$He, which is useful in understanding various superfluid phases of both bulk $^3$He and disordered $^3$He in aerogel.


Anisotropic properties of superfluid $^3$He near free surface studied by surface electrons, Kimitoshi Kono, Hiroki Ikegami, Riken, Low Temperature Physics Laboratory, Riken Team — We performed conductivity measurements of the Wigner solid on the surface of superfluid $^3$He-A and B phases under magnetic fields. The $^3$He-A phase has a nodal point of energy gap at North and South Poles of the Fermi sphere and is anisotropic. A unit vector directing from the South Pole to the North Pole is referred to as the $\ell$ vector. The $\ell$ vector tends to align parallel to a surface normal. The conductivity of the Wigner solid is sensitive to the quasiparticle distribution, and hence, sensitive to the alignment of the $\ell$ vector. Our observation is in good agreement with the abovementioned picture of the $\ell$ vector alignment. In the B-phase the situation is more subtle. Nevertheless, our observation gives a strong support for the present understanding of the magnetic-field-induced anisotropy of the B-phase.

1 Supported by an Alfred P. Sloan Research Fellowship (YL), NSF grants DMR-0239483 (YL) and DMR-0305371 (MWM).

Ultrasonic Propagation in the Normal State of Liquid $^3$He/98% Aerogel, H.C. Choi, N. Masuhara, B.H. Moon, P. Bhupathi, M.W. Meisel, Y. Lee, Microkelvin Laboratory, Department of Physics, U. of Florida, Gainesville, FL 32611, USA, N. Mulders, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716. USA — We studied the propagation of longitudinal sound in the normal state of liquid $^3$He/98% aerogel at 9.5 MHz. The absolute attenuation and sound velocity were determined by direct propagation of sound pulses through the medium. Our measurements cover a wide range of temperatures from 2 mK to 200 mK at three different pressures (10, 21 and 29 bars). As reported by Nomura et al., the sound mode remains in the hydrodynamic limit down to 2 mK due to the impurity scattering off the aerogel. However, we observed a new feature in the high temperature range that the attenuation shows a minimum and increases at high temperature. The minimum $(T_{crit})$ occurs around 60 mK at 10 bars and moves to 40 mK at 29 bars. For $T >> T_{crit}$, the attenuation at high temperature shows a $T^{3.7}$ dependence for all pressures. We will discuss our observations in the framework of theories proposed by Higashitani et al. and Biot.

1 Supported by an Alfred P. Sloan Research Fellowship (YL), NSF grants DMR-0239483 (YL) and DMR-0305371 (MWM).

3:30PM S31.00006 Mass of a quantized vortex, 1, David Thouless, Univ. of Washington, James Anglin, Univ. of Kaiserslautern — There have been many discussions of the mass of quantized vortices in superfluids, but different conclusions have been reached. There is a consensus that vortex mass diverges in compressible superfluids. We have studied the vortex mass in an incompressible quantum fluid by considering a vortex driven slowly round a circular orbit, treating frequency and speed as small parameters. The centrifugal force measures the vortex mass. If a vortex is driven by a large-radius repulsive potential its mass is close to the mass of fluid displaced, as in classical hydrodynamics, but for small pinning radius the mass diverges as the logarithm of the pinning radius. It can be argued that this logarithmic dependence on the pinning radius is a general feature of models of quantized vortices.

1 Partially supported by NSF Award no. DMR-0201948.

3:42PM S31.00007 Vortex stability influenced by surface topology, I. Neumann, P. Voll, N. Aproberts-Warren, P.J. Zieve, UC Davis — We examine the stability of a pinned superfluid helium vortex line. The vortex pins around a thin wire, which terminates at each end at either a rounded bump, a conical indentation, or a flat surface. With the cryostat stationary, we measure the persistence of the vortex. With no external disturbance, it remains indefinitely. We briefly heat the cell and find the temperature at which the vortex depins. By observing the vortex motion after it partially detaches from the wire, we can determine at which terminus it detached. We find that pinning terminating at a bump is generally the easiest to overcome thermally, and pinning at a flat end is the hardest. This pattern would not be expected from considerations of vortex line energy alone. We take the observations as evidence of an additional contribution to the pinning energies. One possibility is an interaction of the vortex with the curvature of the containers surface which favors pinning at points of negative Gaussian curvature, making the bump terminus a less advantageous pin site. The combined effects of vortex line energy and this surface curvature interaction may explain the observed vortex depinning behavior.

Energy Loss from Reconnection with a Vortex Mesh, Rena Zieve, Ingrid Neumann, University of California, Davis — We have observed experimentally that a vortex moving in a cylindrical cell loses energy up to eight orders of magnitude more rapidly than expected from bulk mutual friction alone. Here we investigate the possibility that reconnections with a mesh of small vortices pinned to the cell wall dominate the energy loss. Such pinned vortices may be an unavoidable consequence of rotating the cylinder. Once rotation ceases, most vortices move to the cell wall and annihilate, leaving behind fragments pinned at any microscopic wall roughness. We simulate the situation by requiring the free vortex to move at the local superfluid velocity, and by allowing for reconnections when two vortices approach closely. To keep the simulation run time practical, we use an artificially high friction coefficient. We find that as the vortex moves, reconnections with pinned vortices can reduce its length, and hence its line energy. The energy dissipation of the vortex moving through the mesh can exceed the loss rate from mutual friction by 50% to 100%.
4:06PM S31.00009 Phase-slip avalanches in the superflow of \(^4\text{He}\) through arrays of nano-apertures, David Pekker, Roman Barankov, Paul M. Goldbart, University of Illinois at Urbana Champaign — Recent experiments have explored the dynamics of \(^4\text{He}\) superflow through an array of nano-apertures\cite{1}. These experiments have found that, as the temperature is lowered, phase-slip happens in the apertures changes its character from synchronous to asynchronous. Here, we construct a model\cite{2} of the superflow that incorporates two basic ingredients: (a) disorder associated with each aperture having its own random critical velocity, and (b) an effective inter-aperture coupling, mediated through the bulk superfluid, which stimulates the apertures in the neighborhood of an aperture that has already phase-slipped also to slip. We find that at lower temperatures the synchronicity is lost, due to broadening of the distribution of the critical velocities associated with the reduction of the superfluid healing length. We also observe that as the disorder becomes weak, compared to the inter-aperture coupling, there is a non-equilibrium transition from a regime of small phase-slip avalanches to a regime in which interactions between phase-slips in nearby apertures lead to system-wide phase-slip avalanches.


4:18PM S31.00010 Thinning of superfluid films: critical effects immediately below the \(\lambda\) point, Aviva Shackle, Department of Physics, UCLA, Roya Zandi, Department of Physics, UCR, Joseph Rudnick, Department of Physics, UCLA, Mehran Kardar, Department of Physics, MIT, Lincoln Chayes, Department of Mathematics, UCLA — Experiments on \(^3\text{He}\) films reveal the presence of an attractive Casimir-like force at the bulk \(\lambda\)-point and in the superfluid regime. We address the unexpectedly large magnitude of that force in the regime immediately below the \(\lambda\) point. A simple mean field calculation incorporating the appropriate boundary conditions and adjusted for the renormalizing effects of critical fluctuations points to the source of this dramatic behavior. We find that the location of the minimum of the scaling function is at \(x = LL^{1/\nu} = -\pi^2\) in excellent agreement with the experimental finding of \(x = LL^{1/\nu} = -9.7 \pm 0.8\). Other aspects of the effective force induced by critical fluctuations will also be discussed.

4:30PM S31.00011 Superfluid \(p\)-H\(_2\) Monolayer in Carbon Nanostructures, Milen Kostov, Florida State University — A fluid of para-hydrogen (\(p\)-H\(_2\)) molecules is a prime candidate for potential superfluid, due to the light mass (half the mass of helium) and the existence of a compound boson ground state. In bulk \(p\)-H\(_2\) superfluidity is not observed because, unlike helium, molecular hydrogen solidifies at a temperature (triple point \(T = 13.8\) K) significantly higher than that (\(T = 2\) K) at which such phenomena as Bose Condensation and, possibly, superfluidity (SF) might occur. This is due to the fact that \(H_2\) - \(H_2\) interaction is significantly stronger than the He-He one (more than a factor of three in the well depth). One way to attain a liquid ground state at low \(T\) is to reduce the effective attraction between the \(H_2\) molecules. Here a novel solution to the problem is proposed, which implies that a SF monolayer \(p\)-H\(_2\) can be achieved in a carbon slit-pore with height \(H = 5.8\) Å, where the alignment of the graphitic planes corresponds exactly to the AB stacking sequence in a pristine hexagonal graphite crystal. Our approach is based on the idea to attain a liquid ground state of \(p\)-H\(_2\) monolayer at low \(T\) (\(T = 2\) K), through a substantial renormalization of the pair interaction of \(p\)-H\(_2\) molecules due to their interaction with the surface electrons of the carbon slit pore. In this environment, the resulting de Boer quantum parameter \(\eta\) for the adsorbed \(p\)-H\(_2\) film lies in the vicinity of the threshold value for zero-temperature Bose liquid.

4:42PM S31.00012 Properties of Helium-4 In and Near the Self-Organized Critical State\(^1\), S.T.P. Boyd, D.A. Sergatskov, R.V. Duncan, University of New Mexico — If a downward heat flux is imposed on a sample of \(^4\text{He}\) near \(T_\lambda\), the sample can self-organize so that its temperature tracks the variation of \(T_\lambda\) induced by the hydrostatic pressure head. This “Self-Organized-Critical” (SOC) state is the only means by which a uniform reduced temperature very close to \(T_\lambda\) can be achieved on Earth in \(^4\text{He}\). We recently reported preliminary analysis of extensive new measurements of the SOC state showing three new results: strong nonlinearity in the upward-going wave under high drive levels, the qualitative form of critical fluctuations points to the source of this dramatic behavior. We find that the location of the minimum of the scaling function is at \(x = LL^{1/\nu} = -\pi^2\) in excellent agreement with the experimental finding of \(x = LL^{1/\nu} = -9.7 \pm 0.8\). Other aspects of the effective force induced by critical fluctuations will also be discussed.

\(^1\) work supported in part by NASA.

4:54PM S31.00013 High Tc Magnet Leads for Research Cryostats, Yuko Shiroyanagi, Gokul Gopalakrishnan, Sanghun An, Thomas Gramilla, Ohio State University — The incorporation of high temperature superconducting wires in cryogenic systems has almost exclusively been in those systems with active cryocoolers, or when very high currents are necessary. Despite their obvious advantages, however, various properties of the wires have precluded their use in typical liquid Helium research cryostats. We report here the successful implementation of these wires into a research cryostat magnet lead design, and will discuss design features, aspects of assembly, and characterization of the lead system. The overall design is based on a baffle cooled approach\cite{1} for removing heats from the leads, whose development involved careful numerical modeling. The design approach used for the Hi-Tc magnet lead system leverages this capability to address the various problems associated with superconducting wires, permitting their incorporation.


5:06PM S31.00014 Wave-function approach for a rotating fermionic superfluid, Victor Vakaryuk, UIUC — Rotation of a neutral fermionic superfluid in annular geometry is considered using Gross-Pitaevskii ansatz for the wave function of the system. It is shown that, in the thermodynamic equilibrium, the rotation frequency at which transition between different total angular momentum states occurs is independent on interparticle interactions assuming they are central. The question of whether or not the equilibrium state of a superconductor in a magnetic field corresponds to rotation is also addressed.

Wednesday, March 7, 2007 2:30PM - 5:06PM

Session S41 DCMP: Steps, Facets, and Evolution of Surface Structures 504
**2:30PM S41.00001 Temperature Dependence of the Step Line Tension and Island Decay on the Si(111) (1x1) Surface**, M.S. ALTMAN, K.L. MAN, A.B. PANG, Hong Kong Univ. of Science and Technology, T. STASEVICH, F. SZALMA, T.L. EINSTEIN, Univ. of Maryland — Atomic steps are common defects at surfaces that can play an important role in many phenomena. Advances in the fabrication of nanostructures at surfaces depend largely upon the degree to which one can understand and control factors that affect step morphology. The step line tension is a crucial element in the Gibbs-Thomson relation, which describes the dependence of the chemical potential of an surface step upon its radius of curvature. This dependence can have a notable influence on step morphology. A proper description step morphological phenomena therefore requires accurate knowledge of line tension, including its temperature dependence. The step line tension on the Si(111) (1x1) surface was determined from a capillary wave analysis of two-dimensional island edge fluctuations that were observed with low energy electron microscopy. The line tension decreases by nearly 20% between 1145 K and 1233 K. The role of desorption in island decay varies from negligible to dominant in the temperature range, 1145 – 1380 K, that island decay was measured. A general model of island decay is presented that takes account of desorption. Evaluation of the island decay time with this model referenced to the temperature-dependent line tension accurately determines activation energies that are relevant to island decay and sublimation.

**2:42PM S41.00002 Phase Field Model for Step Dynamics Including Elastic Interactions Between Steps and the Ehrlich-Schwoebel Barrier**, DONG-HEE YEON, KATSUYO THORNTON, R. J. PHANEUF, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109, USA — Understanding the evolution of steps on a vicinal surface is crucial in many important problems involving surfaces. Elastic interactions between steps and the preferential incorporation of adatoms into the upper step due to an asymmetric energy barrier, so-called the Ehrlich-Schwoebel(ES) barrier, greatly influence the step dynamics, often generating morphological instabilities of steps. For example, in the step bunching instabilities, the elastic interactions invoke the progressive coalescence of steps, while the ES barrier has a stabilizing effect. We present a phase-field model for step dynamics including effects of elastic interactions and the ES barrier, and its application to investigate the effects of these factors on step dynamics. The results of the linear stability analysis will also be presented and are compared with those obtained by the phase-field model. In our simulation, it is shown that the flux is an important factor limiting the growth of step bunches through the debunching process. We will also present the analyses of step meandering instabilities resulting from the interplay among the elastic interaction, the ES barrier, and the step line energy.

**2:54PM S41.00003 Distinctive Fluctuations of Facet Edges**, M. DEGAWA, T. J. STASEVICH, W. G. CULLEN, ALBERTO PIMPINELLI, T. L. EINSTEIN, U. of Maryland, College Park — Spurred by theoretical predictions of distinctive static scaling of the step bunching of facets and the extension of these results to dynamic scaling, also rederiving the static results heuristically and we measure this behavior using STM line scans. The correlation functions go as $\phi^{15.5\pm0.3}$ decidedly different from the $\phi^{2.62\pm0.02}$ behavior for fluctuations of isolated steps. From the exponents, we categorize the universality, confirming the prediction that the non-linear term of the KPZ equation, long known to play a central role in non-equilibrium phenomena, can also arise from the curvature or potential-asymmetry contribution to the step free energy. We study a simple model with Monte Carlo simulations to illustrate the novel scaling of fluctuations in an asymmetric potential.

**3:06PM S41.00004 Evolution of patterned step structure on vicinal Si(111) surface during high temperature annealing**, HUNG-CHIH KAN, Department of Physics, University of Maryland, College Park, TAESOOK KWON, RAYMOND PHANEUF, Department of Materials Science and Engineering, University of Maryland, College Park — We present the results of numerical simulations of the evolution of patterned step structures on vicinal Si(111) surfaces during high temperature annealing, which presumably drives the surface far away from equilibrium. We use a mesoscopic model [1] to describe the motion of individual steps under the effects of sublimation, step stiffness (line tension), and step-step interaction. The qualitative consistency between our simulation and experiment [2] suggest that thermodynamic driving force, such as the step-stiffness and step-step interaction dominate the evolution of the step structure during high temperature annealing. [1] J. D. Weeks, D.-J. Lui, and H.-C. Jeong, in Dynamics of step meandering instabilities resulting from the interplay among the elastic interaction, the ES barrier, and the step line energy.

**3:18PM S41.00005 Step Density Minimum on Vicinal Surfaces and Surface Cusps in Epitaxial Regrowth on Patterned Substrates**, TIAN LI, University of Illinois, Urbana, IL, A. BALLESTAD, T. TIEDJE, University of British Columbia, Vancouver, BC — In kinetic Monte Carlo (KMC) simulations of a solid-on-solid model of epitaxial growth, we measure the step density as a function of surface slope and find a special slope where the step density has a minimum. This slope occurs where the surface step density changes from two dimensional (islands) to one dimensional (staircase). The minimum in the step density results from the fact that one dimensional steps are more efficient at capturing adatoms than two dimensional steps, so that a small vicinal angle tends to suppress nucleation of islands. The slope for minimum step density is most sharply defined at low growth rates and high temperatures where the step edges tend to be smooth. The special slope goes away at low temperatures where the steps have a convoluted fractal shape. The minimum in the step density generates characteristic features in KMC simulations for stable (negative Ehrlich Schwoebel barriers) growth on patterned substrates, namely cusps on the top and shoulders of ridges. These features are also found in a continuum growth model which includes the step density minimum. Simulated surface shapes are in good agreement with experimental data for MBE growth of GaAs on patterned substrates, and with data in the literature.

**3:30PM S41.00006 The reconstructions of Si(15 3 23)**, TERESA DAVIES, CRISTIAN CIOBANU, Colorado School of Mines — Among the few remaining puzzles in the physics of heteroepitaxial quantum dots, there remains the atomic structure of the facets that bound the dome-like islands. For a large range of germanium concentrations in the deposited Si-Ge alloy, the (15 3 23) orientation appears to be ubiquitous as the highest-index facet present on the dots at the latest stages of their coherent growth. We present here two approaches to the determination of the reconstructions of Si(15 3 23), one based on a systematic elimination of bonding possibilities and the other being a structural search performed via a genetic algorithm. Both approaches lead to classes of reconstruction models that have much lower surface energies than the only proposal currently available in the literature. Furthermore, the models allow for the presence of low-energy edges between the (15 3 23)-orientations and other facets present on the quantum dots.
3:42PM S41.00007 Faceting of Re (1121) induced by ammonia, supported by DOE-BES

HAO WANG, WENHUA CHEN, THEODORE E. MADEY, Dept. of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854, TIMO JACOB, Fritz-Haber-Institut der MPG, Berlin, Germany — The ammonia-induced nanoscale faceting of Re (1121) has been studied by LEED and STM; the results are compared with recent studies of O-induced faceting of Re(1121). After exposure to ammonia at 700K, the Re(1121) surface only shows a (1×2) reconstruction and remains planar (ammonia dissociates on Re, and only N remains on the surface at T>700K). By exposure to ammonia at 900K, Re(1121) becomes completely faceted, forming 2-sided ridge-like structures with (1342) and (3142) facets. However, this morphology is different from that in O-induced faceting of Re(1121). The two ridge sides, (1342) and (3142), are vicinal surfaces of closed-packed (0110) and (1010) respectively; these latter two surfaces appear as facets in O-induced faceting of Re(1121). DFT calculations are implemented to understand the origin of the different morphologies. Our work demonstrates that it is possible to tailor the surface morphology by choosing appropriate adsorbate and annealing conditions, which in turn provides model systems to study structural sensitivity in catalytic reactions as well as potential templates to grow nanostructures.

3:54PM S41.00008 LEEM study of nucleation, growth, and decay of Ag nanowires on Cu(110), INDRAJITH SENEVIRATHNE, Louisiana State University, EZRA BUSSMANN, GARY KELLOGG, Sandia National Laboratory, RICHARD KURTZ, PHILIP SPRUNGER, Louisiana State University — Low energy electron microscopy (LEEM) has been used to study the nucleation, growth, and ripening of Ag nanowires on Cu(110). Previous STM and LEED studies of Ag on the Cu(110) surface have shown that for a Ag coverage of below 0.3 ML, Ag forms a surface alloy, followed by the formation of a 2D Ag(111) flat superstructure through dealloying at one monolayer. For Ag coverages above 1.3 ML, nanowires of Ag(110), with widths/heights of 12 nm / 2 nm, grow along the [11-21] crystallographic direction with highly anisotropic aspect ratios. LEEM reveals that Ag initially alloys at Cu/Ag step edges producing a distortion of the steps. Upon deposition above 1 ML, nucleation of Ag nanowires was observed across terraces, however nucleation still occurred at defect and step edges. LEEM showed that the nanowires grow to micron lengths and have highly anisotropic aspect ratios. Annealing above 573K resulted in rapid Oswald ripening of nanowires to Ag clusters of several micron dimensions. Further details of the growth and decay mechanisms will be discussed. Sandia is a Lockheed Martin Company, for the US DOE’s NNSA under Contract DE-AC04-94AL85000. Work was supported CINT-U2006A123 and NSF-DMR-0504654.

4:06PM S41.00009 Studies of Cu adatom island ripening on Cu(100) by LEEM, GARY L. KELLOGG, Sandia National Labs — Simple metal surfaces are model systems for characterizing kinetic processes governing the growth and stability of nanoscale structures. It is generally presumed that diffusive transport of adatoms across terraces determines the rate of these processes. However, STM studies in the temperature range T~330-420K reveal that transport between step edges on the Cu(100) surface is limited by detachment barriers at the step edges, rather than by the adatom diffusion barrier. This is because on the Cu(100) surface, mass transport is mediated primarily by vacancies, instead of adatoms. We have used low energy electron microscopy (LEEM) movies to characterize coarsening of Cu islands on the Cu(100) surface in the range T~460-560K. By measuring the temperature dependence of the island decay rate we find an activation barrier of 0.9±0.1 eV. This value is comparable to the 0.8±0.03 eV barrier found in STM studies. However, we are not able to conclude that transport is entirely detachment limited at these elevated temperatures. This work serves as background to establish whether or not Pd alloying in the Cu(100) surface will slow Cu surface transport.

4:18PM S41.00010 Growth of Au on Si(111) surface, A.-L. CHIN, F.-K. MEN, Department of Physics, National Chung Cheng University, Taiwan, ROC — We have studied the growth of sub-monolayer Au atoms on Si(111)-(7×7) surface using scanning tunneling microscopy. By heating the Si substrate after room-temperature Au deposition, we have observed the formation of two types of the (5×2) structure on a (7×7) terrace: one is the (5×2) depressions with an apparent height slightly lower than that of the terrace, the other is the protruding (5×2) unit cell. The surface steps act as good sinks for Au adatoms coming either from the up or down terraces. Widths of denuded zones have been investigated by analyzing the spatial distribution of the (5×2) structure. We will discuss relevant surface diffusion parameters related to the growth of Au.

4:30PM S41.00011 Nucleation, Structure, Morphology of Co on Ag(110): temperature dependent subsurface migration, PHILIP SPRUNGER, INDRAJITH SENEVIRATHNE, Department of Physics and Astronomy, Louisiana State University, ORHAN KIZILKAYA, Center for Advanced Micro Structures and Devices - CAMD, Louisiana State University, RICHARD KURTZ, Department of Physics and Astronomy, Louisiana State University — STM, LEED and Auger spectroscopy have been used to study the nucleation, structure, and morphology of Co on Ag(110) as a function of both coverage and temperature. STM has shown that films grown at coverages of θ < 1ML and low substrate temperatures (~150K) give rise to segregation of Co to the subsurface layer. Furthermore it is possible to observe the nucleation of displaced Ag into small monatomic height islands on top of the substrate. For higher coverages of Co, θ > 1ML a 3-D cluster growth mode takes place giving islands. These islands have a typical ~20 Å diameter and the height of ~3 Å. However, upon annealing the surface to ~673K, profound changes are observed on the morphology of the surface. STM shows that there is a drastic reduction of the density and height of Co islands on the surface, presumably due to subsurface Co cluster growth. Further verification of this was obtained by sequential LEED and Auger spectra obtained while progressive annealing. It was observed the onset of this process occurs at ~673K and flattens out at ~873K. This work is funded by NSF NSF-DMR-0504654.

4:42PM S41.00012 Morphology Evolution of Cobalt Thin Films on Al2O3 (110) Above the Roughening Transition: Formation of Gigantic Multilayered Islands, JORGE ESPINOSA, LEONARDO GOLUBOVIC, DAVID LEDERMAN, Department of Physics, West Virginia University — Co films, 4.0 nm thick, were grown on Al2O3 (110) at 315 °C via molecular beam epitaxy. Their surfaces were imaged via atomic force microscopy while annealing at T ~ 535 °C for several hours. The films exhibited a striking formation of multilayered islands that reach heights more than ten times larger than the initial film thickness. At the early stages of the annealing process (t < 2 hr) the islands’ height h grows exponentially with time t, which is consistent with height instabilities of the film surface. For t > 2 hr, h continues increasing at a slower rate with a power law h ~ t^(γ) with γ = 0.20 – 0.25, whereas, interestingly, the base areas of the multilayer islands do not appreciably change with time. This behavior is independent of t in the 535 °C to 590 °C range. These phenomena are discussed within an interface dynamics model incorporating both surface diffusion relaxation and de-wetting forces. The model is used to elucidate the physical origin of the observed island height growth in terms of strong up-hill surface currents caused by long range Casimir-like forces acting across the film.

1This work was supported in part by the National Science Foundation.
4:54PM S41.00013 First-principles studies of the $\sqrt[7]{7} \times \sqrt[7]{7}$ R19.1° structure of sulfur on the Pd(111) surface. DOMINIC ALFONSO, National Energy Technology Laboratory and Parsons Project Services Inc. — Density functional theory is used to investigate the $\sqrt[7]{7} \times \sqrt[7]{7}$ R19.1° structure of sulfur on the Pd(111) surface. Applying the concepts of first-principles atomistic thermodynamics, we analyze the stability of various $\sqrt[7]{7} \times \sqrt[7]{7}$ models in equilibrium with arbitrary H$_2$ and H$_2$S environment. Among the different models that were considered, the densely packed mixed sulfur-metal overlay structure proposed by Berndt et al. [Surf. Sci. 393, L119 (1997)] was found to be the most energetically favorable. This model consists of arrangement of Pd triangles and pentagons on top of Pd(111) with the sulfur atoms at 3/7 monolayer coverage. The dominant mechanism for sulfur interaction with Pd in the overlay region is the rehybridization of sulfur 3 p and metal 4 d bands. Simulated scanning tunneling microscopy image for this structure shows some similarity with that obtained from experiment. Our study confirms that surface sulfide with no structural resemblance to its bulk counterparts can form on Pd(111).

Wednesday, March 7, 2007 2:30PM - 5:30PM –
Session S42 DCMP: Reactions: Kinetics & Dynamics Colorado Convention Center 505

2:30PM S42.00001 Dissociative and molecular adsorption and recombinative desorption of methylchlorosilanes at the Cu (001) surface. J. LALLO, L.V. GONCHAROVA, A.V. ERMAKOV, B.J. HINCH, Dept. of Chemistry, Rutgers University, D. STRONGIN, Dept. of Chemistry, Temple University — The Direct Synthesis of dichlorodimethylsilane above Cu/Si containing surfaces, is central to the commercial manufacture of many silicone compounds. The atomic scale mechanisms responsible for the high selectivity for dichlorodimethylsilane, vs. other chloromethylsilanes, is poorly understood. As part of a more extensive program we report here on the interactions of chloromethylsilanes with copper. Adsorption of dichlorodimethylsilane on Cu(001) is, at least in part, dissociative. Yet AES indicates non-stoichiometric surface concentrations of Cl and C. This observation, which is apparent in both low (140K) and room temperature exposures, is indicative of a facile recombinative desorption process. Subsequent TPD spectra also indicate the desorption of not only the parent adsorbate, but other species also. Indeed the combined cracking patterns, of simultaneously desorbing species, are inconsistent with solely (CH$_3$)$_2$SiCl$_2$ species. We report on the TPD, AES, and high-resolution helium atom scattering studies of (i) adsorption of methylchlorosilanes, and (ii) their coadsorption with added SiH$_3$. CH$_3$, and Cl species, on Cu(001). Evidence for methyl cracking, and disilane production will be discussed.

2:42PM S42.00002 CO adsorption on a transition metal quantum well system: fcc Co/Cu(100). LEVAN TSKIPURI, HUA YAO, ROBERT BARTYNSKI, Rutgers University — We have examined the unoccupied electronic structure and CO bonding strength on the n-ML fccCo/Cu(100) metallic quantum well (MQW) system using inverse photoemission (IPE) and temperature programmed desorption (TPD), respectively. As-grown Co films exhibit well-defined MQW states that disperse upward with increasing film thickness, but they do not cross the Fermi level and are less pronounce than on other similar systems owing to partial overlap of exchange split states. Upon CO adsorption a well-defined structure centered about 3.8 eV above the Fermi level appears and is assigned to the unoccupied CO 2π* orbital. CO adsorbs molecularly at room temperature and in TPD measurements we find a desorption temperature of $\sim 375$ K, which is about $30$ K lower than what is observed for CO adsorbed on the hcp Co surfaces. When Co films are dosed at low temperatures ($\sim 120$ K), we find a second CO desorption peak around 230 K, once again similar to what is seen for hcp Co, but at a markedly lower temperature. We have observed similar desorption peak temperature shifts for CO desorption from the Ni/Cu(100) system. The CO desorption temperature varies with Co layer thickness and the possible role of quantum size effects on the molecule-surface bond will be discussed.

2:54PM S42.00003 The influence of overlap interactions on chemical reactions in confinement. ERIK E. SANTISO, KEITH E. GUBBINS, Center for High Performance Simulation (ChiPS) and Department of Chemical and Biomolecular Engineering, North Carolina State University, AARON M. GEORGE, MARCO BUONGIORNO NARDELLI, Center for High Performance Simulation (ChiPS) and Department of Physics, North Carolina State University — Chemical reactions are often carried out in nano-structured materials due to their large surface area per unit mass. It is, however, difficult to understand fully the role of the nano-structure in many reactions due to the superposition of multiple effects. Such effects include: the reduced dimensionality of the system, the heterogeneity of the pore surfaces, the selective adsorption of reactants/products, catalytic effects, and transport limitations. Experimental studies often show many of these effects at the same time, making the results difficult to interpret. In this work we present results of density functional theory calculations illustrating the influence of overlap interactions (shape-catalytic effects) on chemical reactions. In particular, we show the effect of confinement in small pores on the rates of rotational isomerizations of n-butane, 1-butene and 1,3-butadiene. We find that the rates of these transitions change as the double exponential of the pore size in the molecular sieving limit. These results are a first step towards an integrated model for the effect of confinement in small pores on the rates of rotational isomerizations of n-butane, 1-butene and 1,3-butadiene. We find that the rates of these transitions change as the double exponential of the pore size in the molecular sieving limit. These results are a first step towards an integrated model for the design of catalytic materials.

3:06PM S42.00004 Reactions of water molecules at the Si/SiO2 interface. I.G. BATYREV, L. TSETSERIS, Department of Physics and Astronomy, D.M. FLEETWOOD, R.D. SCHIRMPF, Electrical Engineering and Computer Science, S.T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235 — Water molecules can be present in nanoscale structures due to their large surface area per unit mass. It is, however, difficult to understand fully the role of the nano-structure in many reactions due to the superposition of multiple effects. Such effects include: the reduced dimensionality of the system, the heterogeneity of the pore surfaces, the selective adsorption of reactants/products, catalytic effects, and transport limitations. Experimental studies often show many of these effects at the same time, making the results difficult to interpret. In this work we present results of density functional theory calculations illustrating the influence of overlap interactions (shape-catalytic effects) on chemical reactions. In particular, we show the effect of confinement in small pores on the rates of rotational isomerizations of n-butane, 1-butene and 1,3-butadiene. We find that the rates of these transitions change as the double exponential of the pore size in the molecular sieving limit. These results are a first step towards an integrated model for the design of catalytic materials.

3:18PM S42.00005 Growth kinetic of perovskite oxide monolayers on SrTiO$_3$(100) studied with reflection high energy electron diffraction (RHEED) and oblique-incidence optical reflectivity difference measurements. XU WANG, YIYAN FEI, XIANGDONG ZHU, Department of Physics, University of California at Davis — Using a combination of RHEED and an oblique-incidence optical reflectivity difference technique (OI-RD, a form of polarization modulated ellipsometry), we studied the growth of 5% doped Nb: SrTiO$_3$ monolayers on SrTiO$_3$(100) under pulsed laser deposition condition (PLD) in a molecular oxygen ambient. By interrupting the deposition at the completion of one monolayer and continuing the RHEED and OI-RD measurement during post-deposition annealing, we can separate contributions to the optical reflectivity difference signal from kinetics of growth and chemical reactivity. Based on a mean-field theory of optical reflectivity difference off an atomically rough and yet optically smooth film, we find that a growth-dependent part of the reflectivity difference signal is proportional to the step edge density or equivalently the root-mean-square (rms) of the roughness of a growth surface. We show that the surface roughness during the interrupted deposition of Nb: SrTiO$_3$ monolayers on SrTiO$_3$(100) can be analyzed with a 8-level growth model with two adjustable parameters. The parameters obtained by fitting the model to the OI-RD signal during the interrupted deposition can be used subsequently to predict the growth behaviour of Nb: SrTiO$_3$ on SrTiO$_3$(100) in a continuous pulsed laser deposition as reported earlier by Fei and co-workers.
3:30PM  S42.00006 Grating-coupled excitation and detection of surface plasmon polariton waves (SPPW) on Cu(111) using periodic density patterns of rare gas monolayers. , YIYAN FEI, XU WANG, XIANGDONG ZHU, Department of Physics, University of California at Davis — Using periodic density profiles of xenon (Xe) as thin as 1 ~ 5 monolayers, we have excited and detected grating-coupled surface plasmon polariton waves (SPPW) on Cu(111) in ultrahigh vacuum. The periodic density profiles are formed by laser-induced thermal desorption with a pair of coherent laser pulses at vacuum wavelength of 0.532 µm. The periodicity of the profiles is 5.45 µm. By illuminating the xenon-density-grating-covered Cu(111) with a converging He-Ne laser covering a span of incidence angles from 66.4° to 74.4° and detecting the oblique-incidence reflectivity difference \( r_p/r_o = r_{p1}/r_{o1} \) vs. incidence angle with a multiple-element photodiode array, we observed the surface-plasmon resonance (SPR) peaked at \( \phi_{SPR} = 74.4° \) with a full-width at half-maximum \( \Delta \phi_{SPR} = 0.29° \). From the resonance angle \( \phi_{SPR} \) and \( \Delta \phi_{SPR} \), we have determined the optical dielectric constant of single crystalline Cu at 633 nm to be \( \varepsilon_{Cu} = -9.53 + i 0.142 \), markedly different from the literature values for evaporated Cu films. At elevated temperatures such that a xenon density grating on Cu(111) decays in contrast, the surface plasmon resonance as measured by \( r_p/r_o \) - \( r_{p1}/r_{o1} \) diminishes, reflecting the kinetic surface diffusion of xenon on Cu(111).

3:42PM  S42.00007 STM-induced passivation of Si (100) surface from physisorbed molecular hydrogen at 5 K , AMENA L. KHAN, ALLAN R. MACDAIRD, DAVID C. FORTIN, XIAOBIN ZHU, MARK R. FREEMAN, Department of Physics, University of Alberta, Edmonton, Canada T6G 2G7 — Gas phase adsorption of hydrogen on silicon surfaces is usually achieved through reaction with molecular hydrogen at elevated temperatures and/or exposure of the surface to atomic hydrogen.[1] In the present work, we introduce molecular hydrogen to a silicon (100) surface at T = 5 K. In these conditions we observe physisorption of molecular hydrogen, [2] which can act as a precursor for the formation of hydrides on the silicon surface. It is found that scanning tunneling microscopy can be used to induce patterned chemisorption of hydrogen on silicon. Upon repetitive scanning of the same area at negative sample bias, complete passivation of the area can be achieved. The route to complete termination involves two stages, the second of which appears to proceed via nucleation and growth of completely terminated islands from within a disordered, partially terminated phase. At positive sample bias the second stage is not observed, with the induced chemisorption ending in an unreactive “locked” configuration of the surface still containing silicon dangling bonds. This work is supported by NSERC, iCORE and CIAR. References: [1] A. J. Mayne, D. Riedel, G. Comtet, G. Dujardin, Prog. Surf. Sci., 81, 1, 2006. [2] T. R. Govers, L. Mattera, G. Scoles, J. Phys. Chem., 72, 5446, 1980

3:54PM  S42.00008 Quantum Size Effects on Surface Catalysis from First-Principles Studies . LI HUANG, School of Physics, Georgia Institute of Technology; Ames Laboratory, XINGAO GONG, Physics Department, Fudan University, ZHENYU ZHANG, Materials Science and Technology Division, Oak Ridge National Laboratory — Using first-principles calculations within density functional theory, we find that the adsorption energies and diffusion barriers of O and CO on quantum (Au+Ag) films show thickness-dependent oscillations. Such oscillations are solely determined by the total thickness of the (Au+Ag) films. The synergetic standing waves formed in the films due to quantum confinement and interference give rise to such quantum oscillation. This result points to potential tunability of the chemical reactivity on ultrathin metal films.

4:06PM  S42.00009 Theoretical investigation of CO oxidation on AuAg (110) alloy surface. , JHY PIN CHOU, IAMS, Academia Sinica, Taipei, Taiwan and National Chung Cheng University, Chia-Yi, Taiwan, CHING-MING WELI, IAMS, Academia Sinica, Taipei, Taiwan — Carbon monoxide (CO) oxidation on the gold-silver (110) binary alloy surface has been investigated by using density functional theory. For clean metal (110) surface, it was found that CO prefers to adsorb on atop and short bridge site of Au(110) surface [1] and O2 prefers to adsorb on fourfold hollow (FFH) site of Ag(110) surface [2]. In this work, we present the results of CO, O2 adsorption, and CO+O2 coadsorption on AuAg(110) surface. The results indicate that the adsorption energy is mainly determined by the type of atoms on the bonding site. For CO, adsorption on Au atop and Au2 short bridge site are favored and have an adsorption energy range of 0.43–0.63 eV. For O2 adsorption on FFH site with Au5−nAgn, (n=3) configuration is possible and has an adsorption energy range of 0.12–0.53 eV. For CO+O2 coadsorption, the coadsorption energy on Au−Ag(110) is slightly less than the sum of CO and O2 adsorption energy by only 0.05–0.1 eV. The oxidation of adsorbed CO with O2 is found to proceed via formation of an intermediate, OC(O), and has a surprising low energy barrier of 0.2–0.3 eV. [1] Tatyana E. Shubina, Christoph Harting and Marc T. M. Koper, Phys. Chem. Chem. Phys. 6, 4215,(2004) [2] P. A. Gravil and D. M. Bird, Phys. Rev. Lett. 77, 3993(1996)

4:18PM  S42.00010 What is Special in Silver for Ethyene Epoxidation , PAOLA GAVA, SISSA − Scuola Internazionale Superiore di Studi Avanzati e CNR-INFN DEMOCRITOS National Simulation Center, I-34014 Trieste, Italy, ANTON KOKALJ, Jožef Stefan Institute, SI-1000 Ljubljana, Slovenia, STEFANO DE GIRONCOLI, SISSA − Scuola Internazionale Superiore di Studi Avanzati e CNR-INFN DEMOCRITOS National Simulation Center, I-34014 Trieste, Italy, STEFANO BARONI1 — We present a first-principles study of Ethylene Oxide (EO) synthesis on different transition and noble metal surfaces. Recently Linic et al. have shown that on silver ethylene oxametallacycle (OMC) is a common intermediate for EO as well as for acetaldehyde (Ac) formation, the latter leading to undesired total combustion [1]. Our results provide a rationale of these findings which stem from the mild reactivity of silver that hinders H–C and C–C bond breaking both in ethylene and in the OMC intermediate. By analyzing the transition state geometries toward EO and Ac we identify an indicator that strongly correlates with selectivity for EO formation and could be a useful tool in the rational search for an improved catalyst. [1] S. Linic et al., J. Am. Chem. Soc. 125, 4034 (2003)

3:40PM  S42.00011 CS radical formation in the Hot Filament CVD of diamond thin film by the CRDS , MADALINA BUZAIANU, University of Puerto Rico, Dept. of Physics, VLADIMIR MAKAROV, University of Puerto Rico, Dept. of Chemistry, ARTURO Hidalgo, University of Puerto Rico, Dept. of Physics, BRAD WEINER, University of Puerto Rico, Dept. of Chemistry, GERARDO MORELL, University of Puerto Rico, Dept. of Physics — In the present study, the CS radical was detected using Cavity Ringdown Spectroscopic (CRDS) during the Hot Filament CVD growth of diamond thin film for the CH4 / H2 mixture doped with H2S. The absolute absorption optical density of the CS radical was obtained, and the concentration of this radical was estimated as function of CH4 and H2S concentrations. It was found that the yield of the CS radical depends on the presence of the substrate. The experimental results show that the heterogeneous sources of the CS radical are more significant in the presence of the substrate than in experiments without substrate. The relationship between the homogeneous and heterogeneous channels of the CS radical generation was estimated for both cases with and without substrate. The translational (Doppler analysis of the line contour) and rotational (fitting of the rotationally resolved CS spectrum) temperatures were estimated.
4:42PM S42.00012 High Pressure and High Temperature Decomposition Studies of PETN and TATB, MICHAEL PRAVICA, HUBERTUS GIEFERS, EDWARD ROMANO, University of Nevada, Las Vegas and High Pressure Science and Engineering Center (HIPSEC), BRIAN YULGA, University of Nevada, Las Vegas and High Pressure Science and Engineering Center (HIPSEC), ZACHARY QUINE, University of Nevada, Las Vegas and High Pressure Science and Engineering Center (HIPSEC), WENGE YANG, High Pressure Collaborative Access Team (HP-CAT), Advanced Photon Source and the Carnegie Geophysical Institution, HANS PETER LIERMANN, High Pressure Collaborative Access Team (HP-CAT), Advanced Photon Source, and the Carnegie Geophysical Institution — We present a variety of high pressure and high temperature studies investigating radiation-induced decomposition of the high explosives PETN and TATB using white beam synchrotron radiation at the Advanced Photon Source. Diffraction line intensities were measured as a function of time using energy-dispersive techniques. By measuring the decomposition rate as a function of pressure and temperature, kinetic and other constants associated with the decomposition reaction were extracted.

4:54PM S42.00013 Investigation of the SH formation mechanism in Hot Filament CVD of diamond thin film by CRDS, VLADIMIR MAKAROV, University of Puerto Rico, Dept. of Chemistry, MADALINA BUZAIANU, ARTURO HIDALGO, University of Puerto Rico, Dept. of Physics, BRAD WEINER, University of Puerto Rico, Dept. of Chemistry, GERARDO MORELL, University of Puerto Rico, Dept. of Physics — The SH radical formation mechanism during the Hot Filament CVD (HFCVD) of diamond thin film was studied using Cavity Ringdown Spectroscopy (CRDS) for the CH$_4$ / H$_2$ mixture upon addition of traces amounts of H$_2$S. The absorption spectrum of the SH radical as function of different parameters (filmament material, distance between filament and probing laser area of CRD cell, CH$_4$ and H$_2$S concentrations, presence and absence of substrate) was studied. The gas temperature and the SH concentration profiles were obtained. The SH radical yield saturates for CH$_4$ concentrations higher than 4 %. From the analysis of the experimental data we expect to understand the sources and the decay channels related to the mechanism of the SH radical formation during the HFCVD of the diamond thin film. The SH translational (Doppler analysis of the line countur), rotational (rotationally resolved spectrum fitting) and vibrational (measurement of the relative populations of SH on the ν'' = 0 and ν'' = 1 vibronic states) temperatures were estimated.

5:06PM S42.00014 Investigation of the Role of Surface Oxides in Catalysis by Gold Nanoparticles, HONGGOING SHI, CATHERINE STAMPFL, The University of Sydney, Sydney, Australia — In contrast to the long held view that gold is catalytically inert, it is now well known that supported gold nanoparticles are notably more active than other transition metals for low temperature catalytic oxidation of CO. Through density-functional theory and the approach of inert, it is now well known that supported gold nanoparticles are notably more active than other transition metals for low temperature catalytic oxidation of CO, and as well as promoting several other catalytic reactions [1]. This has stimulated huge efforts in an attempt to understand the mechanisms responsible for the high activity, including investigations into the nature of oxygen on gold surfaces [2]. Through density-functional theory and the approach of ab initio thermodynamics [3] we have found that on the gold (111) surface, thin oxide-like structures are significantly more stable for the pressure and temperature conditions of CO oxidation. The energetic preference for such partially oxidized gold, is in accord with very recent experimental results [4]. For the identified lowest energy surface oxide-like structure, we investigate the adsorption of CO on the surface and determine the reaction pathways for CO oxidation.

5:18PM S42.00015 Modeling the effect of adsorbates on the surface segregation of binary alloy surfaces, OLE M. LØVVIK, University of Oslo, SUSANNE M. OPALKA, United Technologies Research Center — The effect of adsorbed species on surface segregation in binary alloys has been investigated using band-structure density-functional theory. Particular emphasis is given to hydrogen adsorption on the Pd-Ag and Pd-Cu systems, which are of relevance for hydrogen selective dense metal membranes. It is demonstrated how adsorption can significantly alter the atomic-scale surface segregation in such binary alloy surfaces.

Wednesday, March 7, 2007 2:30PM - 5:18PM – Session S43 DCMP: Photonic Crystals Colorado Convention Center 506

2:30PM S43.00001 Theory of Band Structure of Thin Photonic Crystals1, JEFFREY SOKOLOFF, Northern University — There exist several highly successful methods for calculating the band structure of thick photonic crystals (PC’s), constructed from parallel dielectric rods, which are long compared to their diameters and spacings. None of these methods, however, can accurately calculate the band structure of the technologically important case of thin PC’s (i.e., PC’s consisting of a periodic array of dielectric rods or holes in a dielectric material of length comparable to or smaller than the hole or rod diameter and spacing). Methods analogous to approximate methods traditionally used to calculate the band structure of crystalline solids, such as the tight binding method (where the rods or holes which are resonant cavities play the role of atoms) or the augmented plane wave method will be applied to this problem. The resulting band structure for thin PC’s is much different from that of thick PC’s. For example, there exist lower/higher frequency flat bands, resulting from the tight binding functions constructed from linear combinations of the resonant modes of the rods/holes.

2:42PM S43.00002 Quasi-phase-matched Cerenkov radiation generation in a two-dimensional nonlinear photonic crystal waveguide, S. N. ZHU, Y. ZHANG, Z. QI, G. ZHAO, W. WANG, Nanjing University, NATIONAL LABORATORY OF SOLID STATE MICROSTRUCTURES & PHYSICS DEPARTMENT TEAM — In this report, we present a new type of quasi-phase-matched Cerenkov radiation generation from a two-dimensional nonlinear photonic crystal waveguide: a hexagonally poled LiTaO$_3$ waveguide. The waveguide was fabricated by field poling followed by proton exchange technique. The fundamental source was a LD-pumped, 90-ns pulsed Q-switch double wavelength Nd:YAG laser at 1064-μm and 1319-μm. The pulse repetition rates were 8-KHz. When the fundamental beams at 1064-μm and 1319-μm were collinearly focused into the waveguide and propagated along its x-axis, three sets of hexagonal patterns, with red, yellow and green colors, were respectively exhibited on the projection screen behind the waveguide at the same time. They were confirmed to be the second-harmonic generation (red and green patterns) and sum-frequency generation (yellow pattern) for these two fundamental waves, respectively. These frequency conversion processes were realized by guided-to-radiated mode interaction. Phase-matching for these processes in the waveguide was automatically achieved by a quasi-phase-matched Cerenkov configuration.

1 Airforce Research Laboratories contract number FA8-718-06-C-0045
2:54PM S43.00003 Optical spectra in Fibonacci photonic nanostructures1, E.L. ALBUQUERQUE, F.F. DE MEDEIROS, L.R. DA SILVA, Departamento de Física, Universidade Federal do Rio Grande do Norte, 59072-970, Natal-RN, Brazil — In this work, we have studied the transmission spectra of photonic band-gap Fibonacci quasiperiodic nanostructures composed of both positive (SiO₂) and negative refractive index (n) materials, the so-called metamaterials. These left-handed materials has been receiving recently a lot of attention due to their novel properties, like the possibility of the construction of perfect lenses. Also, the mirror symmetry structure is very sensitive to the phase compensation effect, which is unique in the positive and negative refractive index stacked Fibonacci nanostructures. The transmission spectra of these Fibonacci nanostructures, for the case where both refractive index can be approximated as a constant, show a sharp Fano-type resonance that is well observed due to its internal coupling between localized modes and propagation modes, enabling the structure to be used as an ideal optical filter. For more realistic case, where the permittivity is modelled by a plasmonic dielectric function, there is no more a self-similar pattern, although keeping Bragg refraction gaps. In both cases, however, our transmission spectra unveil smooth structure due to the phase compensation effect, including the so-called zero-n gap case.

3:06PM S43.00004 Thermal emission from two-dimensional metallo-dielectric photonic crystals, MOHIT DIWEKAR, Z.V. VARDENY, University of Utah, Department of Physics, Salt Lake City, Utah 84112 — We studied thermal light emission from a sub-wavelength hole arrays with square lattice of 4 μm periodicity fabricated in aluminum (Al) and silver (Ag) films on silicon (Si) substrates by conventional photolithography. The emission spectra were obtained using a FTIR setup with a port for an external cryostat configured for thermal emission measurements. These patterned films show extraordinary transmission bands in the mid-IR spectral range, which can be well explained as due to light coupling to surface plasmons on the two film interfaces. The thermal emission spectrum from these photonic crystals followed the transmission spectrum characteristics; however it differs significantly from the obtained absorption spectrum, in contrast to the Kirchhoff’s law of radiation. We conclude that the fabricated photonic structures behave as radiation filters where the emission radiation is suppressed in the frequency range outside the transmission bands in the spectrum.

3:18PM S43.00005 Berry phase for optical wavepacket propagation in deformed photonic crystals, KEI SAWADA, SHUICHI MURAKAMI, NAOTO NAGAOSA, CREST, Department of Applied Physics, the University of Tokyo — We develop a theory for a trajectory of an optical wavepacket propagating through a photonic crystal with a deformation [1]. Naively one might expect that the trajectory of an optical beam is always perpendicular to the wave front, which is expected in a conventional geometrical optics derived from Fermat’s principle. We reveal an anomalous behavior of such electromagnetic beams beyond this naive expectation. We derive a set of equations motion which includes multiple scatterings and a geometrical phase called Berry phase associated with the wave dynamics. We find that such a Berry phase correction to geometrical optics gives rise to a shift of the center position of an wavepacket. Remarkably, at the edge of a photonic band gap, such a coordinate shift is enhanced by a factor \( \Delta \omega / \omega \), where \( \omega \) is a frequency of light and \( \Delta \omega \) is a size of a photonic band gap. An amount of the enhancement factor is \( \omega / \Delta \omega \approx 10^2 \) for photonic crystals. Especially, in the case of an x-ray dynamical diffraction, the factor can be \( \omega / \Delta \omega \approx 10^9 \), which implies that an atomic crystal deformation gives a macroscopic shift of a wavepacket.

1We thank financial support from CNPq-Rede NanoBioEstruturas.

3:30PM S43.00006 Terahertz transmission of single-mode photonic crystal slabs1, CRISTO YEE, NATHAN JUKAM, MARK SHERWIN, Physics Dept., University of California Santa Barbara — Terahertz (THz) radiation lies in the gap between optical and electronic frequencies. Its importance has grown during the past few years due to applications ranging from security to quantum information processing. These applications often require manipulating electromagnetic radiation on-chip, and THz Photonic Crystals (PC) are a natural solution. Terahertz PCs have two advantage: Silicon has a negligible absorption and the large PC dimensions makes fabrication defects negligible. In this work we report the first measurement of a transmission through a single mode THz PC Slab. The PC slab was fabricated with Reactive Ion Etching on a high-resistivity Si wafer. The PC slab was fabricated using a 2D triangular array of holes with lattice constant \( a = 0.64 \ mu \) m, radius \( r = 0.3 \ mu \) m and thickness \( d = 0.74a \). The PC slab was fabricated with Reactive Ion Etching on a high-resistivity Si wafer. FTIR transmission spectrum along the J orientation shows an optical bangap from 1.2 to 1.6 THz for the TE mode, in good agreement with our FDTD calculations. The PC slab is the starting point for testing devices like waveguides and cavities.

1This work was supported by NSF grant CCF0507295 and CONACYT-UCMEXUS.

3:42PM S43.00007 Multi-layered photonic crystals de novo: new formalism, results, insights, and analytic possibilities1, FRANK SZMULOWICZ, University of Dayton Research Institute — A new formalism for calculating the photonic band structure of multi-layer photonic gap (PBG) materials is derived. The formalism expresses all boundary conditions in terms of tangents rather than exponential functions. The formalism is compact, algorithmically simple, and physically appealing, and provides a new conceptual framework for describing the photonic band structure of layered materials. Its simplicity makes it possible to represent eigenfrequency conditions using geometric constructs, finding a factored form of the secular equation, and derive analytic eigenfrequency conditions and analytic wave functions for multi-layer structures. Computationally, the new formalism makes it possible to find explicitly the complete band structure of multi-layer PBG materials with integer ratios of optical path lengths (e.g., any combination of quarter-wave, half-wave, etc., stacks) through a single diagonalization of a low order secular equation, the alternative being an implicit root search via the transfer matrix formalism. The formalism is demonstrated on multi-layered structures arranged in the Fibonacci sequence and half-wave-quarter-wave-eighth-wave PBG.

1This work was supported by the Air Force Contract FA8650-06-D-5401 at the Materials & Manufacturing Directorate, AFRL/ML.

3:54PM S43.00008 The Rayleigh Hypothesis and Scattering at Photonic Crystal Surfaces1, PRABASAJ PAUL, KYAW NYEIN, ROBERT CHOUDURY, Denison University — We examine the Rayleigh hypothesis in the context of scattering of light off photonic crystal interfaces. First, the hypothesis – which was initially suggested for scattering of waves off rough surfaces between homogeneous media – is rephrased to apply to photonic crystal interfaces. Next, some exact and explicit functional forms are presented that map plane photonic crystal surfaces to periodic rough surfaces in free space, so that known criteria for the validity of the Rayleigh hypothesis for scattering at rough surfaces can be applied directly to scattering at the photonic crystal surfaces. The same maps also allow the scattering problem to be solved exactly. We present numerical results for scattering amplitudes at a photonic crystal surface using both the exact method (based on a surface integral formulation) and an approximate method (based on the Rayleigh hypothesis). The results are found to be consistent with the analytical criteria for the range of validity of the approximate method.

1Supported in part by the Research Corporation.
4:06PM S43.00009 Optical Characterization of 3D Photonic Crystals Fabricated by Holographic Lithography1, YING-CHIEH CHEN, JOSEPH B. GEDDES III, PAUL V. BRAUN, PIERRE WILTZIUS, Department of Materials Science and Engineering, Beckman Institute, University of Illinois at Urbana-Champaign — Holographic lithography is a promising technique for fabricating photonic crystals. Due to the large area, defect-free nature of the crystals created, they are expected to be good model systems for the study of their optical properties. However, the crystals created experimentally do not always meet theoretical expectations. We will present our current understanding of the optical response by comparing the experimental and simulated optical spectra. These spectra were taken from holographically fabricated crystals having FCC geometry. Optical spectra were simulated using a frequency domain algorithm for both the ideal photonic crystal and cross-sectional SEM images from the fabricated crystals as inputs to the simulation. Experimental issues associated with inconsistencies between measured and predicted results of the optical response will be discussed.

1This work is supported by MURI grant # DAAD19-03-1-0227.

4:18PM S43.00010 Tunable Mesoporous Defects in Photonic Crystals, F.C. PEIRIS, J.R. RODRIGUEZ, Physics, Kenyon College, V. KITAEV, Chemistry, Wilfred Laurier Uni., G.A. OZIN, Chemistry, Un. Toronto — Similar to doping in semiconductors, the incorporation of defects into photonic crystals introduces defect-based states in the photonic bad gap, resulting in an increase in its functionality. In this work, we have introduced a planar-defect into a colloidal photonic crystal, and have investigated the evolution of its optical properties with respect to the infiltration of various foreign constituents. A periodic mesoporous silica film (i.e., the defect) was deposited on a silica-based colloidal photonic crystal, and a second photonic crystal was deposited subsequently to encompass the defect-layer. UV-VIS spectroscopy, scanning electron microscopy and X-ray diffraction experiments confirm the existence of the meso-layer. Subsequently, water vapor and tetramethyl orthosilicate (TMOS) were infiltrated into the structure and the defect-based signature corresponding to the optical spectra was monitored. In both cases, a noticeable shift in wavelength was observed, providing evidence that the structure performs as a chemical sensor.

4:30PM S43.00011 Robust Optimization of Aperiodic Photonic Structures1, OMID NOHADANI, KWONG MENG TEO, DIMITRIS BERTSIMAS, Massachusetts Institute of Technology — In engineering design, the physical properties of a system can often only be described by numerical simulation. Optimization of such systems is usually accomplished heuristically without taking into account that there are implementation errors that lead to very suboptimal, and often, infeasible solutions. We present a novel robust optimization method for electromagnetic scattering problems with large degrees of freedom, and report on results when this technique is applied to optimization of aperiodic dielectric structures. The spatial configuration of 50 dielectric scattering cylinders is optimized to match a desired target function such that the optimal arrangement is robust against placement and prototype errors. Our optimization method inherently improves the robustness of the optimized solution with respect to relevant errors and is suitable for real-world design of materials with novel electromagnetic functionalities.

1supported by DARPA.

4:42PM S43.00012 Enhanced and Tailored Emission from Luminescent Three-Dimensional Ru(bpy)$_3$(PF$_6$)$_2$ Inverse-Opal Photonic Crystals, ANDREW BRZEZINSKI, JYH-TSUNG LEE, University of Illinois at Urbana-Champaign, JASON SLinker, Cornell University, Ithaca, NY, PIERRE WILTZIUS, University of Illinois at Urbana-Champaign, GEORGE MALLIARAS, Cornell University, Ithaca, NY, PAUL BRAUN, University of Illinois at Urbana-Champaign — Three-dimensional inverse opal structures, with various lattice constants are made by infilling polystyrene colloid templates with luminescent Ru(bpy)$_3$(PF$_6$)$_2$. The passive photoluminescent structures and active electroluminescent organic light-emitting-diode structures were characterized via electron microscopy and solid-angle-resolved spectroscopy. A model is presented, explaining light propagation within and emission from the crystal. Results show angular emission profiles are tailored by choice of lattice constant, which determines directions in which light is emitted. Enhanced emissive flux is achieved by suppressing propagation in near parallel directions relative to the air interface.

4:54PM S43.00013 Negative refractions of acoustic waves in sonic crystals1, YAN-FENG CHEN, MING-HUI LU, LIANG FENG, YONG-YUAN ZHU, SHI-NING ZHU, NAI-BEN MING, Nanjing University, MICROSTRUCTURED MATERIALS TEAM2 — Acoustic wave exhibits inherently different characters when propagating in sonic band-gap materials in which their elastic constants are modulated in order of acoustic wavelength. We present negative refraction of acoustic wave both experimentally and theoretically in two dimensional sonic crystals constructed with steel rods embedded in air. With lattice symmetry and artificial atoms? design, refraction of acoustic wave in the crystals could be manipulated from positive to negative and from defocusing to focusing with sonic crystal plates. Acoustic band structures, analogy to electron band structure in semiconductors and photonic band structure in photonic crystals, attribute to these abundant characters of acoustic waves propagation.

1Supported by 973 projects and NSFC.
2National Lab. of Solid-State Microstructures

5:06PM S43.00014 A direct time integration of Maxwell equations in dielectric and magnetic dispersive materials for FDTD modelling of metamaterials, JESUS MANZANARES-MARTINEZ, JORGE GASPARR-ARMENTA, Departamento de Investigacion en Fisica, Universidad de Sonora — A new procedure of integration for the Maxwell equations is present to study dielectric and magnetic dispersive materials using the Finite Difference Time Domain Method. Our method is based on a direct application of the Fourier Transform for the temporal and frequency integrations of the constitutive relations. We study Drude and Lorentz dispersive media. We present different results for the light reflection of a pulse impinging dispersive dielectric, dispersive magnetic, or both dispersive media.

Thursday, March 8, 2007 8:00AM - 10:24AM –
Session U1 DCMP: RNA Folding at the Crossroads Between Molecular Biology and Statistical Physics
Colorado Convention Center Four Seasons 2-3

8:00AM U1.00001 Topological classification of RNA pseudoknots, TONY ZEE, University of California at Santa Barbara — No abstract available.
8:36AM U1.00002 Aggregation and folding phase transitions of RNA molecules1, RALF BUNDSCUH, The Ohio State University — RNA is a biomolecule that is involved in nearly all aspects of cellular functions. In order to perform many of these functions, RNA molecules have to fold into specific secondary structures. This folding is driven by the tendency of the bases to form Watson-Crick base pairs. Beyond the biological importance of RNA, the relatively simple rules for structure formation of RNA make it a very interesting system from the statistical physics point of view. We will present examples of phase transitions in RNA secondary structure formation that are amenable to analytical descriptions. A special focus will be on aggregation between several RNA molecules which is important for some regulatory circuits based on RNA structure, triplet repeat diseases like Huntington’s, and as a model for prion diseases. We show that depending on the relative strength of the intramolecular and the intermolecular base pairing, RNA molecules undergo a transition into an aggregated phase and quantitatively characterize this transition.

This work has been partially supported by the National Science foundation through grant no. DMR-0404615.

9:12AM U1.00003 Ground state and glass transition of the RNA secondary structure1, LEI-HAN TANG, Hong Kong Baptist University — RNA molecules form a sequence-specific self-pairing pattern at low temperatures. Understanding the relevant energy scales that govern sequence specificity is important for thermal and mutational stability studies of functional RNAs. This problem has been analyzed using a random pairing energy model as well as a random sequence model that includes a base stacking energy in favor of helix propagation [1]. The free energy cost for separating a chain into two equal halves offers a quantitative measure of sequence specific pairing [2]. In the low temperature glass phase, this quantity is shown to grow quadratically with the logarithm of the chain length, but it switches to a linear behavior of entropic origin in the high temperature molten phase. Numerical studies of the melting transition suggest similarities to the thermal depinning of a two-dimensional elastic manifold in a disordered medium, though details of the analogy need to be further explored. For designed sequences, however, a power-law distribution of pairing energies on a coarse-grained level may be more appropriate. Extreme value statistics arguments then predict a power-law growth of the free energy cost to break a chain, in agreement with numerical simulations. Interestingly, the distribution of pairing distances in the ground state secondary structure follows a remarkable power-law with an exponent 4/3, independent of specific assumptions for the base pairing energies.

1Research is supported in part by the RGC of the HKSAR under grant 2601/01P.

9:48AM U1.00004 Glassiness in RNA folding, KAY J. WIESE, LPT ENS, Paris — We study secondary structures of random RNA molecules by means of a renormalized field theory based on an expansion in the sequence disorder. We show that there is a continuous phase transition from a molten phase at higher temperatures to a low-temperature glass phase. Based on an exact inequality, we argue that RNA conformations in the glass phase are similar to those at the transition.


Thursday, March 8, 2007 8:00AM - 11:00AM — Session U2 GQI DCMP: Quantum Cryptography and Quantum Communication I

8:00AM U2.00001 Entanglement-Based Quantum Cryptography and Quantum Communication1, ANTON ZEILINGER, University of Vienna, Austria — Quantum entanglement, to Erwin Schroedinger the essential feature of quantum mechanics, has become a central resource in various quantum communication protocols including quantum cryptography and quantum teleportation. From a fundamental point of view what is exploited in these experiments is the very fact which led Schroedinger to his statement namely that in entangled states joint properties of the entangled systems may be well defined while the individual subsystems may carry no information at all. In entanglement-based quantum cryptography it leads to the most elegant possible solution of the classic key distribution problem. It implies that the key comes into existence at spatially distant location at the same time and does not need to be transported. A number recent developments include for example highly efficient, robust and stable sources of entangled photons with a broad bandwidth of desired features. Also, entanglement-based quantum cryptography is successfully joining other methods in the work towards demonstrating quantum key distribution networks. Along that line recently decoy-state quantum cryptography over a distance of 144 km between two Canary Islands was demonstrated successfully. Such experiments also open up the possibility of quantum communication on a really large scale using LEO satellites. Another important possible future branch of quantum communication involves quantum repeaters in order to cover larger distances with entangled states. Recently the connection of two fully independent lasers in an entanglement swapping experiment did demonstrate that the timing control of such systems on a femtosecond time scale is possible. A related development includes recent demonstrations of all-optical one-way quantum computation schemes with the extremely short cycle time of only 100 nanoseconds.

1Work supported by ARO, DTO, the European Commission and by FWF.

8:36AM U2.00002 Beller Lectureship Recipient Talk: Applications of Quantum Teleportation2, JIANWEI PAN, Physikalisches Institut der Universitaet Heidelberg, Germany and Hefei National Laboratory for Physical Sciences at Microscale, China — Quantum teleportation, a way to transfer the state of a quantum system from one location to another, is central to quantum communication and plays an important role in a number of quantum computation protocols. Previous experimental demonstrations have been implemented with single photonic or ionic qubits. Very recently long-distance teleportation and open-destination teleportation have also been realized. Until now, previous experiments have only been able to teleport single qubits. However, since teleportation of single qubits is insufficient for a large-scale realization of quantum communication and computation, teleportation of a composite system containing two or more qubits has been seen as a long-standing goal in quantum information science. In my talk, I shall present the first experimental realization of quantum teleportation of a two-qubit composite system. In the experiment, we develop and exploit a six-photon interferometer to teleport an arbitrary polarization state of two photons. Not only does our six-photon interferometer provide an important step towards teleportation of a complex system, it will also enable future experimental investigations on a number of fundamental quantum communication and computation protocols such as multi-stage realization of quantum-relay, fault-tolerant quantum computation, universal quantum error-correction and one-way quantum computation.

2This work was supported by the Marie Curie Excellent Grant of the EU and the Alexander von Humboldt Foundation. This work was also supported by the National Natural Science Foundation of China and the Chinese Academy of Sciences.
9:12AM U2.00003 Twenty two years of quantum key distribution. RICHARD HUGHES, Los Alamos National Laboratory — Following their 1984 invention of quantum key distribution (QKD), Bennett and Brassard and colleagues performed a proof-of-principle QKD transmission over a 32-cm air path in 1991. This seminal experiment led other researchers to explore implementations of QKD in optical fibers and over line-of-sight outdoor atmospheric paths (“free-space”), resulting in dramatic increases in range, secret bit rate, security and availability. These advances have led to, and been enabled by, improvements in sources, single-photon detectors and the deeper understanding of QKD security with practical sources and detectors in the presence of transmission loss and channel noise. Today, QKD has been implemented with unconditional security over ranges greater than 100km, over multi-kilometer distances in high background environments in both fiber and free-space, and at high (GHz) clock rates over shorter distances. In my talk I will review the key enabling advances underlying these developments of experimental optical fiber and free-space QKD over the past 15 years, describe the present status of the field, and compare and contrast different approaches to implementing security against photon number splitting attacks. I will describe some recent results from QKD in dedicated (“dark”) optical fiber using ultra-high efficiency, low-noise transition edge sensor (TES) photo-detectors, achieving ultra-long transmission distances, and unconditional security over 107km through the use of a decoy-state protocol. I will also describe progress in making QKD compatible with all-optical fiber networks, including the co-existence of QKD signals with conventional optical data on the same fiber. I will conclude my talk with a survey of the prospects for QKD transmission distances exceeding 200km, which will include a comparison of the various single-photon detector technologies now becoming available for quantum communications.

9:48AM U2.00004 Security of Quantum Key Distribution. NORBERT LÜTKENHAUS, Institute for Quantum Computing, Department of Physics & Astronomy, University of Waterloo — Quantum Key Distribution (QKD) is the most advanced application of Quantum Information Science. It allows extending secret keys over some distances in such a way that the security of the resulting key material can be guaranteed by the laws of quantum mechanics. In contrast to presently used encryption techniques, the security of QKD can be proven in terms of information-theoretic measures. The resulting key can then be used for many tasks, including exchanging secret messages. QKD has been developed in the language of abstract two-level systems, the qubits. They cannot be easily implemented in optical signals. It took some time to bring the protocols and theory of QKD to the point where they fit to the realities of fiber-optical or free-space applications, including lossy channels. Today, QKD schemes can be implemented reliably using standard off-the-shelf components. Information-theoretic security is a theoretical concept. Naturally, it is impossible to demonstrate directly that a given experimental set-up indeed creates a secret key. What one can do is to show that the experiment can give data within a certain parameters regime, such as error rate and loss rate, for which a security proof exists. I will discuss what parameter regime gives provable secret key and which parameter regime cannot lead to secret key. It is desirable to prove ‘unconditional security,’ as it is termed in the world of classical cryptography: no assumption is made about the attacks of an eavesdropper on the quantum channel. However, one has to assume that the signal structure and the measurement device are correctly described by the adopted model and that no eavesdropper can intrude the sender or receiver unit. In this talk I will briefly introduce the concept of QKD and optical implementations. Especially I will discuss security aspects of modern approaches of QKD schemes that allow us to increase the covered distance and the achievable rate.

10:24AM U2.00005 Towards a practical quantum repeater, ALEX KUZMICH, Georgia Institute of Technology — Quantum mechanics provides a mechanism for absolutely secure communication between remote parties. For distances greater than 100 kilometers direct quantum communication via optical fiber is not viable, due to fiber losses, and intermediate storage of the quantum information along the transmission channel is necessary. This lead to the concept of the quantum repeater, proposed in 1998 by Briegel, Duer, Cirac, and Zoller. In 2001, Duan, Lukin, Cirac, and Zoller have proposed to use atomic ensembles as the basic memory elements for the quantum repeater. We will outline our program on the use of atomic ensembles as an interface for quantum information transfer and the prospects for long distance quantum networks.

Thursday, March 8, 2007 8:00AM - 11:00AM — Session U3 DCMP: Quantum Chaos in Condensed Matter Physics Colorado Convention Center Korbel 2A-3A

8:00AM U3.00001 Single-Channel Scattering from Disordered Samples: a sensitive probe of the eigenfunctions behavior. YAN FYODOROV, University of Nottingham — The goal of the talk is to demonstrate that that statistics of waves reflected from a disordered sample via a single open channel can serve as a sensitive probe of the eigenfunctions behaviour inside the sample in all regimes: localized, extended, and critical (multifractal). In particular, it allows one to understand the anomalous scaling exponents governing the multifractal behavior of the moments of the Wigner time delay at the point of the Anderson localization transition. The method also reveals some nontrivial exact symmetry relations which must be satisfied by the anomalous exponents and multifractality spectra. These predictions were recently verified in accurate numerical simulations.

8:36AM U3.00002 Scattering fidelity in random matrix elastodynamics, the effect of temperature on diffuse ultrasound\textsuperscript{1}. RICHARD L. WEAVER, University of Illinois — Temperature variations in a high Q elastic body provide access to a slowly and reversibly tuned wave chaotic random ultrasound “Hamiltonian.” This allows benchtop measurements of scattering fidelity in quantum chaotic, and other, systems. To a first approximation, temperature changes merely rescale time, as the wave speeds and specimen size change. But inasmuch as the shear and longitudinal wave speeds change by different amounts, the wave fields are distorted as well. The degree of distortion is a measure of how rapidly the shear and longitudinal waves mix. We show how that distortion varies with temperature, with the age of a transient waveform, with frequency, and with specimen size and geometry. Measured scattering fidelities are found to be in accord with predictions from random matrix theory for both irregular and regular bodies, up to a scaling parameter that is related to the rate of mixing of the rays. That rate is very different depending on the regularity of the specimen. Fidelity is greater in ray-chaotic bodies than in regular bodies.

\textsuperscript{1} Work supported by the NSF CMS 05-28096
9:12AM U3.00003 Analog Experiments on Quantum Chaotic Scattering and Transport¹, STEVEN ANLAGE, University of Maryland — The transport properties of mesoscopic and nanoscopic materials are dominated by quantum interference effects. Nevertheless it is challenging to delineate these effects through conventional transport experiments on real materials. Complications arise from finite temperatures (thermal smearing, inelastic scattering), and the excitation of two-level systems that can cause the electrons to “decouple” and drop out of the quantum-coherent transport process. We approach this problem from the perspective of nonlinear dynamics and utilize a unique experimental technique that directly simulates the quantum scattering properties of complicated (ray-chaotic) systems. A microwave cavity is used to simulate solutions to the time-independent Schrödinger equation for a two-dimensional ray-chaotic infinite square-well potential. The classically chaotic ray trajectories within a suitably shaped microwave cavity play a role analogous to that of the chaotic dynamics of noninteracting electron transport through a ballistic quantum dot in the absence of thermal fluctuations. In wave chaotic scattering, statistical fluctuations of the scattering matrix $S$ and the impendence (‘reaction’) matrix $Z$ depend both on universal properties and on nonuniversal details of how the scatterer is coupled to external channels. We remove the non-universal effects of the coupling from the experimental data using the radiation impedance obtained directly from the experiments, thus eliminating one of the most significant complications in conventional transport measurements. The Landauer-Büttiker formalism is applied to obtain the conductance of a corresponding mesoscopic quantum-dot device. We find good agreement for the probability density functions of the experimentally derived surrogate conductance, as well as its mean and variance, with the theoretical predictions based on random matrix theory [1]. We also observe a linear relation between the quantum dephasing parameter and the cavity ohmic loss parameter. The results apply to scattering measurements on any wave chaotic system. We also discuss future directions for this work.

¹This work is done in collaboration with Thomas Antonsen, James Hart, Sameer Hemmady, Edward Ott, and Xing Zheng, and is supported by the AFOSR MURI and DURIP programs.

9:48AM U3.00004 Quantum Networks as Models of Mesoscopic Systems, TSAMPIKOS KOTTOS, Department of Physics, Wesleyan University, Connecticut-USA and MPI for Dynamics and Self-Organization, Göttingen-Germany — We review our work on quantum networks. These are one-dimensional systems consisting of vertices connected by bonds that have incommensurate lengths $L$. Particles with a fixed wave-number $k$ can propagate freely on the bonds and scatter at the vertices. Combining the free propagation and the vertex scattering we have ended up with a quantum “evolution” operator on the graph. The corresponding classical dynamics was defined as follows: we have constructed a Liouville description by considering the evolution of a phase-space density over the space of directed bonds. The classical evolution operator consists of transition probabilities between connected bonds taken from the corresponding quantum evolution operator. Due to the multiple connectivity (stretching) and the compactness of the system (folding), the classical dynamics is chaotic. This analogy enables us to study the connection between statistical properties of eigenvalues and eigenfunctions and the classical dynamics. Finally, connecting them with leads to infinity we also know that quantum networks are excellent paradigms for the study of mesoscopic transport.

10:24AM U3.00005 The classical limit of quantum transport¹, SAAR RAHAV, University of Maryland — Weak localization and conductance fluctuations are manifestations of quantum interference on transport. These quantum effects take a finite time, the Ehrenfest time, to appear. We present a semiclassical calculation of the Ehrenfest time dependence of weak localization and conductance fluctuations for ballistic quantum dots. Weak localization is found to be suppressed when the Ehrenfest time is larger than the typical dwell time in the dot. In contrast, the conductance fluctuations are found to be Ehrenfest time independent. The calculated Ehrenfest time dependences are consistent with numerical results.

¹Work done in collaboration with Piet W. Brouwer, Cornell University.

Thursday, March 8, 2007 8:00AM - 11:00AM – Session U10 DCMP: Charge Density Waves and 1D Systems

8:00AM U10.00001 A Kadanoff-Wilson renormalization group analysis of half-filled one-dimensional quantum electron-phonon models, HASSAN BAKRIM, CLAUDE BOURBONNAIS, Departement de physique, Universite de Sherbrooke, Sherbrooke, Quebec, Canada J1K-2R1 — We study the zero temperature phase diagrams of the half-filled one-dimensional Su-Schrieffer-Heeger (SSH) and molecular crystal (CM) models using the Kadanoff-Wilson renormalization group approach. At the one-loop level, the full frequency dependence of the phonon induced electron-electron coupling constants is taken into account in the vertex corrections and the quantum interference between the Cooper and Peierls diffusion channels. This enters as a key ingredient for the description of the quantum to classical transition for the Peierls instability. Our results confirm that finite phonon frequency introduces quantum fluctuations that depress the Peierls gap $\Delta$ compared to the classical - mean field - limit $\Delta_0$. It is found that in the spinless fermion case, the Peierls gap vanishes at the threshold $\omega_{\xi} / \pi \Delta_0$, whereas for fermions with spins, the gap remains in the quantum spin-charge separated regime. We extend our study to the XY spin-Peierls chain and confirm the DMRG result about the existence of a power law relation between the critical spin-phonon coupling $\alpha$, and frequency at the quantum-classical boundary, namely $\alpha_c \sim \omega_{\xi}^{-7}$. 

8:12AM U10.00002 Small Bipolarons in the anisotropic 2-dimensional Holstein-Hubbard model, JUN ZHOU, JEROME DORIGNAC, DAVID CAMPBELL, Boston University — We will investigate the bipolaron states in the anisotropic two-dimensional Holstein-Hubbard model. The interplay between attractive electron-phonon coupling $g$ and the repulsive electron-electron interaction $v$ will generate many different ground states. The anisotropic electron hopping in two dimensions also plays a role in affecting the bipolaron state. The bipolaron could be located on a single site or be two polarons separated by several sites or a quasidiscrete state which is the superposition of 4 electronic singlets with a common central site.

8:24AM U10.00003 Fermi surface pockets and Luttinger sum rule in low-dimensional systems¹, CHRISTOPHE BERTHOD, THIERRY GIAMARCHI, DPMC, University of Geneva, Switzerland, SILKE BIERMANN, ANTOINE GEORGES, CNRS-UMR, Ecole Polytechnique, France — We investigate the Mott transition in a quasi-one dimensional system of weakly coupled interacting fermionic chains. Within a generalization of dynamic mean field theory, we study by quantum Monte Carlo the evolution of the electron self-energy with increasing inter-chain coupling. Our approach is able to capture the closing of the Mott gap at some critical coupling, and is thus ideally suited to examine the characteristics of the Mott transition in this and similar systems. We find that the transition proceeds through an intermediate phase where the Fermi surface is broken into electron and hole pockets. Although these pockets can be very small, we show that the Luttinger sum rule is obeyed throughout the phase diagram.

8:36AM U10.00004 Does nesting really cause Charge Density Waves? , MICHELLE JOHANNES, IGOR MAZIN, Naval Research Laboratory, Washington, D.C. — The concept of a CDW induced by Fermi-surface nesting originated from the Peierls idea of electronic instabilities in purely 1D metals and is now often applied to charge ordering in real, low-dimensional materials. The idea is that Fermi surface contours coincide when shifted along the observed CDW wave vector, then the CDW is considered to be nesting-derived. We argue that only a tiny fraction, if any, of the observed charge ordering phase transitions are true analogues of the Peierls instability, i.e. that (a) there is substantial nesting of the FS, as quantified by a peak in Im \chi_0(q) at the CDW wave vector; (b) this peak translates (as in the 1D case) into a peak in \Re\chi_0(q) at the same wave vector; (c) a divergence in the full electronic susceptibility causes the electronic subsystem to be unstable without ion shifts; and (d) all phonons are softened at the CDW vector. Using prototypical CDW materials NbSe\textsubscript{2}, NbSe\textsubscript{3}, and CeTe\textsubscript{3}, we show that these conditions are hardly ever fulfilled, and that the CDW phases are actually structural phase transitions, driven by ionic rather than electronic instabilities. We also show mathematically that the original Peierls construction is so fragile as to be unlikely to apply to any real material.

8:48AM U10.00005 The pseudogap phase in \((\text{TaSe}_3)_2\)\textsubscript{I}, ANDRAS VANYOLOSL, BALAZS DORA, ATTILA VIROSZTEK, Department of Physics, Budapest University of Technology and Economics, 1521 Budapest, Hungary — We have developed the mean-field theory of coexisting charge-density-wave (CDW) and unconventional charge-density-wave (UCDW). The double phase transition manifests itself in the thermodynamic quantities and in the magnetic response, such as spin susceptibility and nuclear spin-lattice relaxation rate. Our theory qualitatively applies to the quasi-one dimensional CDW material \((\text{TaSe}_3)_2\)\textsubscript{I}. This material exhibits peculiar properties: above the CDW transition temperature \(T_c\), thermal fluctuations were found to die out rapidly, but robust pseudogap behavior is still detected. Namely, the experimental findings include: (i) sharp increase of the static spin susceptibility above \(T_c\), (ii) smooth increase of the spin-lattice relaxation rate above \(T_c\), (iii) as opposed to conventional CDW, no sharp feature in the spin-lattice relaxation rate below \(T_c\). We have found that our coexisting CDW+UCDW model qualitatively describes these observed properties of \((\text{TaSe}_3)_2\)\textsubscript{I}. Direct calculations for the magnetic response are shown to evidence the agreement. We also argue, that the fluctuations around \(T_c\) are suppressed due to the presence of the “hidden” UCDW phase, which partially gaps the Fermi surface, and causes non-Fermi-liquid (pseudogap) behavior.

9:00AM U10.00006 Charge density wave formation and physical properties of \(R_2\text{Te}_5\) \((R=\text{Nd, Gd})\) compounds, K. Y. SHIN, N. RU, Geballe Laboratory for Advanced Materials and Department of Applied Physics, Stanford University, Stanford, California 94305, USA, M. F. TONEY, Stanford Synchrotron Radiation Laboratory, Stanford Linear Accelerator Center, 2575 Sand Hill Road, Menlo Park, California 94025, USA, I. R. FISHER, Geballe Laboratory for Advanced Materials and Department of Applied Physics, Stanford University, Stanford, California 94305, USA — \(R_2\text{Te}_5\) \((R=\text{Nd, Gd})\) has a layered tetragonal structure based on alternating single and double square planar Te sheets separated by corrugated \(R\text{Te}\) layers, and has a quasi-two dimensional electronic structure. The material shares important physical properties with other two single and double Te layer variants, \(R\text{Te}_2\) and \(R\text{Te}_3\) \((R=\text{La, Yb})\), including a charge density wave (CDW) instability. Using a binary self-flux method, we have grown high-quality single crystals of \(\text{Gd}_2\text{Te}_3\) and \(\text{Nd}_2\text{Te}_3\) compounds and have characterized their structural, thermodynamic and transport properties. Our measurements reveal, for the first time, the charge density wave in this material. We will discuss the properties and origin of the CDW, and the relation to the better known \(R\text{Te}_2\) and \(R\text{Te}_3\) compounds.

9:12AM U10.00007 Effect of Chemical Pressure on the Charge Density Wave Transition in Rare-earth Tritellurides \(R\text{Te}_3\), N. RU, Dept. of Applied Physics, Geballe Lab. for Adv. Materials, Stanford University, G. Y. MARGULIS, Dept. of Physics, Geballe Lab. for Adv. Materials, Stanford University, K. Y. SHIN, Dept. of Applied Physics, Geballe Lab. for Adv. Materials, Stanford University, M. F. TONEY, Stanford Synchrotron Radiation Laboratory, Stanford Linear Accelerator Center, I. R. FISHER, Dept. of Applied Physics, Geballe Lab. for Adv. Materials, Stanford University — The charge density wave transition is investigated in the bi-layer family of rare earth tritelluride \(R\text{Te}_3\) compounds \((R = \text{Sm, Gd, Tb, Dy, Ho, Er, Tm})\) via high resolution x-ray diffraction and electrical resistivity. The transition temperature \(T_{\text{CDW}}\) increases monotonically with increasing lattice parameter by an extraordinarily large amount, from 244(3) K for \(\text{TmTe}_3\) to 416(3) K for \(\text{SmTe}_3\). It is suggested that this behavior, and the observation of a secondary transition for the heaviest members of the series, is intimately linked to the effect of chemical pressure on the degree of bilayer instability in purely 1D metals and is now often applied to charge ordering in real, low-dimensional materials. The idea is that if Fermi surface contours coincide when shifted along the observed CDW wave vector, then the CDW is considered to be nesting-derived. We argue that only a tiny fraction, if any, of the observed charge ordering phase transitions are true analogues of the Peierls instability, i.e. that (a) there is substantial nesting of the FS, as quantified by a peak in Im \chi_0(q) at the CDW wave vector; (b) this peak translates (as in the 1D case) into a peak in \Re\chi_0(q) at the same wave vector; (c) a divergence in the full electronic susceptibility causes the electronic subsystem to be unstable without ion shifts; and (d) all phonons are softened at the CDW vector. Using prototypical CDW materials NbSe\textsubscript{2}, NbSe\textsubscript{3}, and CeTe\textsubscript{3}, we show that these conditions are hardly ever fulfilled, and that the CDW phases are actually structural phase transitions, driven by ionic rather than electronic instabilities. We also show mathematically that the original Peierls construction is so fragile as to be unlikely to apply to any real material.

9:24AM U10.00008 High-resolution STM imaging and spectroscopy of \(\text{Cu}_2\text{TiSe}_2\), DALE KITCHEN, KENJIRO K. GOMES, ABHAY PASUPATHY, AAKASH PUSHHP, PEDRAM ROUSHAN, Princeton Nanocale Microscopy Laboratory, Department of Physics, Princeton University, EMILIA MOROSAN, ROBERT J. CAVA, Department of Chemistry, Princeton University, ALI YAZDANI, Princeton Nanocale Microscopy Laboratory, Department of Physics, Princeton University — The discovery of superconductivity in Cu-doped \(\text{TiSe}_2\) has created a new opportunity to study the competition between charge density wave (CDW) formation and superconductivity in layered chalcogenides [1]. Using a cryogenic scanning tunneling microscope (STM), we have obtained atomic resolution images of \(\text{in situ} \text{ cleaved Cu}_2\text{TiSe}_2\) and perform spatially resolved mapping of the electronic states of this compound. The STM images measured on samples at low Cu doping, reveal the atomic lattice, the CDW organization, and show local signatures consistent with individual Cu-dopants. Imaging and spectroscopy are used to identify how the Cu-dopants alter the local electronic structure of this material and destroy the CDW organization, which eventually gives way to the rise of superconductivity. [1] E. Morosan et al., Nature Physics 2, 544 (2006).

9:36AM U10.00009 STM Studies of the CDW System \(\text{TbTe}_3\), ALAN FANG, ZHANYBEK ALPICHSHEV, NANCY RU, IAN FISHER, AHARON KAPITULNIK, Stanford University — We present STM data on the Charge Density Wave (CDW) in the Rare Earth Tri-Telluride \(\text{TbTe}_3\). Topography scans as large as 250×250 Å\textsuperscript{2} were taken with voltage bias as high as 0.8 Volt. Fourier analysis shows an incommensurate unidirectional modulation with wave-vector \(q \approx 0.71\) a*\textsuperscript{–1}. The topographic scans at different bias voltages are used to highlight the difference in structure of the CDW and lattice period-doubling effects, either from the Te–Te dimerization, or from the Te–Tb layer directly below the surface.

1 This work is supported by the DOE, Office of Basic Energy Sciences, under Contract No. DE-AC03-76SF00515.

2 This work is supported by the Department of Energy, Office of Basic Energy Sciences under contract DE-AC02-76SF00515.

3 Work supported by NSF-MRSEC through PCCM.
9:48AM U10.00010 APRES study of a complex charge density wave material Gd$_2$Te$_3$1. RUIHUA HE, KYUNG YUN SHIN, HONG YAO, Applied Physics & Physics, Stanford University & SSRL, JUDE LAVEROCK, STEPHEN DUGDALE, Department of Physics, University of Bristol, UK, NANCY RU, DONGHUI LU, WORAWAT MEEVASANA, STEVE KIVELSON, IAN FISHER, ZHI-XUN SHEN, Applied Physics & Physics, Stanford University & SSRL — By using angle-resolved photoemission spectroscopy based on synchrotron radiation as well as monochromatic He-I UV, we have investigated for the first time a complex charge density wave (CDW) material, Gd$_2$Te$_3$, of the rare earth (R) telluride family R$_2$Te$_3$, with hybrid crystalline structure of its two well-studied relatives, RTe$_2$ and RT$_2$. Based on a tight-binding model, combining with the LDA calculation, we analyze the experimental Fermi surface, energy band dispersions and their temperature dependence in detail, which provides valuable insights into its complex CDW phase revealed recently by the TEM and XRD measurements. The nature of different CDW wave vectors involved and the roles of different interlayer split bands in the CDW formation are discussed.

1The work at SSRL is supported by DOE’s Office of Basic Energy Sciences under Contracts No. DE-AC02-76SF00515. The work at Stanford is supported by NSF DMR-0604701. R.H. would like to acknowledge the support by Stanford Graduate Fellowship.

10:00AM U10.00011 Electronic Structure and CDW Physics in LaTe$_3$ using ARPES. DANIEL GARCIA, University of California, Berkeley, GEY-HONG GWEON, University of California, Santa Cruz, SHUYUN ZHOU, University of California, Berkeley, JEFFGRAF, Lawrence Berkeley National Laboratory, CHRIS JOZWIAK, University of California, Berkeley, MYUNG-HWA JUNG, Korea Basic Science Institute (KBSI), YONG SEUNG KWONG, Sung Kyun Kwan University, Korea, ALESSANDRA LANZARA, University of California, Berkeley — We report a direct study of the band structure and charge density wave (CDW) formation in LaTe$_3$, by using high-resolution angle-resolved photoemission spectroscopy (ARPES). The nature of the CDW formation, the momentum dependence of the CDW gap and the role of dimensionality in the tellurides will be presented. Finally the transition from a stripe to a checkerboard phase and its layer dependence will be addressed.

10:12AM U10.00012 Doping (x)- and pressure-dependence of the CDW state in Cu$_x$TiSe$_2$ using inelastic light scattering1. HARINIBARATH, MINJUNG KIM, S.L. COOPER, Dept. of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, EMILIA MOROSAN, R.J. CAVA, Department of Chemistry, Princeton University, Princeton, NJ 08540, USA — TiSe$_2$ has long been known to form a rather simple commensurate charge-density-wave (CDW) below $T_{CDW}$ ~ 200K. Interest in this material has grown recently, however, with the discovery that Cu intercalation between the TiSe$_2$ layers [1] suppresses the CDW transition, and at intermediate compositions ($x \approx 0.04$ in Cu$_x$TiSe$_2$), gives rise to a superconducting state. Consequently, Cu$_x$TiSe$_2$ is a particularly interesting system in which to investigate the competition between CDW and superconducting correlations. In this talk, we discuss our inelastic light scattering studies of the effects of chemical tuning on the CDW state in Cu$_x$TiSe$_2$, which we compare to pressure-dependent studies of the CDW state in TiSe$_2$. By monitoring both the CDW amplitude modes and phonons with chemical substitution and pressure, we are able to sensitively study the different routes to CDW melting in this interesting system. [1]. E. Morosan et al., Nature Physics 2, 544 (2006).

1Work supported by the Dept. of Energy under grant No. DEFG02-91ER45439.

10:24AM U10.00013 Using the atomic pair distribution function (PDF) to probe the local structural aspects of charge-density-wave (CDW) state in complex materials. HYUNJEONG KIM, EMIL BOZIN, CHRISTOS MALLIKAS, MERCOURI KANATZIDIS, SIMON BILLINGE, Michigan State University, BOGDAN DABROWSKI, Northern Illinois University, MATTHIAS GUTMANN, ISIS Facility, CCLRC Rutherford Appleton Laboratory — The atomic pair distribution function (PDF) analysis [1], based on total scattering approach, is used to study the CDW state, one of the fundamental broken-symmetry ground-states of metals, commonly found in complex materials. Incommensurate CDW (IC-CDW) found in 2-D tellurium square-net in CeTe$_3$ is a simple single-q CDW driven by Fermi-surface nesting. Our recent PDF study on local distortions in CeTe$_3$ suggests that the IC-CDW in CeTe$_3$ at 300K consists of commensurate CDW domains separated by discommensurations, rather than being a uniform incommensurate CDW as seen crystallographically [2]. Recent PDF results of a study of the local Peierls distortions in isostructural compounds SmTe$_3$ and HoTe$_3$ will be presented. The PDF analysis has also been extended to probe the CDW state in K doped BaBiO$_3$, and a report on the current state of this study will be provided. [1]. T. Egami & S. J. L. Billinge, Underneath the Bragg Peaks: Structural Analysis of Complex Materials, Pergamon Press Elsevier, Oxford, England, 2003 [2]. H. J. Kim et al., Phys. Rev. Lett. 96, 226401 (2006).

10:36AM U10.00014 CDW dynamics in NbSe$_3$ probed by $^{93}$N NMR1. S. SUH, UCLA, P. MONCEAU, CRTBT, CNRS, W. G. CLARK, UCLA, R. E. THORNE, Cornell, S. E. BROWN, UCLA — Using $^{93}$N NMR spin echo experiments on a single crystal of NbSe$_3$, we have probed electric-field induced displacements of the CDW forming below $T_{c}=144K$. In our experiments, good S/N was achieved by aligning the chain axis of a single large crystal (cross-section O(500){m}^2) with the coil symmetry axis. Evidence for CDW motion throughout the sample for $E > E_{F}$ was observed in motional narrowing experiments. For $E \leq 0.9E_{F}$, we find a wide distribution of displacements less than one CDW wavelength, for both unipolar and bipolar electric field pulse excitations. At $E \sim 0.9E_{F}$, the mean displacement is approximately 6-7 degrees, and the width of the distribution is about twice the mean displacement. We discuss the results in the context of the Fukuyama-Lee phase Hamiltonian, and describe the constraints imposed by these experiments on the proposal that CDW depinning is an example of a dynamic critical phenomenon.

1NSF DMR-0520552

10:48AM U10.00015 Transmission Electron Microscopy of Charge Density Wave Transitions of rare-earth transition-metal silicide R$_x$Ir$_{10}$Si$_{10}$ (R=Dy, Ho) . C.H. CHEN, C.M. TSEN, Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan, H.D. YANG, Department of Physics, National Sun-Yat-Sen University, Kaohsiung, Taiwan — The metallic ternary rare-earth transition-metal silicides of R$_x$Ir$_{10}$Si$_{10}$, where $R = \{\text{Dy, Ho}\}$, exhibit charge density wave (CDW) transitions despite its seemingly three-dimensional crystal structure. In this talk we present the observation of the CDW phase transitions in this class of materials by electron diffraction and electron microscopy. These compounds exhibit incommensurate to commensurate phase transitions as temperature decreases. The modulation wave vector is found to be along the c-axis of the crystal with a modulation periodicity approximately four times of the unit cell. Real space imaging of CDW domains and/or domain walls using the dark-field technique in transmission electron microscopy will also be presented.

Thursday, March 8, 2007 8:00AM - 11:00AM – Session U23 DCMP: Low-D Metals and Responses Colorado Convention Center 110
8:00AM U23.00001 Internal friction of a one micron thick silver film between 1 mK and 1 K, ANDREW FEFFERMAN, R. O. POHL, J. M. PARPIA, Cornell University — Metal films are useful for thermalization and electrostatic actuation of both macroscopic and nanoscale oscillators at low temperatures. However, the effect of the metal film on the dynamics of the oscillator substrate is not always known since previous measurements of the internal friction $Q^{-1}$ of metal films extend down to a few hundred mK. Measurements of X. Liu et al [Phys. Rev. B 59, 11767 (1999)] showed that between 0.5 and 1 K many micron-thick metal films exhibit a $Q^{-1}$ plateau at the level of several $10^{-4}$, but the existence of the plateau below 500 mK was unknown. We have measured $Q^{-1}$ of a one micron thick silver film between 1 mK and 1 K using a single crystal silicon double-ended acoustic resonator. The results suggest that $Q^{-1}$ of the film alone could be extracted from measurements of the composite oscillator. $Q^{-1}$ of the silver film was nearly constant at $4 \times 10^{-9}$ between 1 and 10 mK and increased to $10^{-4}$ as temperature increased from 10 mK to 1 K. These data will be valuable for future experiments on metal coated silicon or silicon nitride resonators at mK temperatures.

3Research supported by the NSF under DMR - 0457533 and DARPA

8:12AM U23.00002 Thermal Expansion and Specific Heat of some BeCu Alloys, J.C. COOLEY, J.C. LASHLEY, T.J. TUCKER, W.L. HULTS, S.J. TRACY, G.M. SCHMIEDESCHOFF, Los Alamos National Laboratory — We have measured the specific heat and thermal expansion of some polycrystalline BeCu alloys with an atomic concentration of Cu up to 3%. We will present and discuss our measurements in the context of a Gruneisen analysis.

8:24AM U23.00003 Optical properties of Al at shock-melted conditions, LORIN X. BENEDICT, JOHN E. KLEPEIS, Lawrence Livermore National Lab — We report calculations of the linear optical absorption spectra of aluminum at pressures of roughly 1 Mbar and temperatures of around 5000 K. The calculations, done using a combination of density functional theory and a semi-empirical approach, show that the calculated optical properties are in agreement with both previous measurements and theoretical predictions. The optical properties are found to be sensitive to the pressure and temperature conditions, with the absorption coefficient increasing with increasing temperature and decreasing with increasing pressure.

8:36AM U23.00004 Ultrafast Extreme Ultraviolet Holography: Dynamic Measurement of Surface Deformation, MARK SIEMENS, OREN COHEN, QING LI, MARGARET MURNANE, HENRY KAPTEYN, University of Colorado, JILA, RA’ANAN TOBEY, University of Oxford, KEITH NELSON, Massachusetts Institute of Technology — We demonstrate femtosecond time-resolved dynamic holography using coherent extreme ultraviolet (EUV) light generated by high harmonic upconversion of a femtosecond laser. We use a novel excitation geometry in which a pump laser excites a narrow line on the sample, and a much larger EUV beam probes the perturbed sample. The unperturbed portion of the sample reflects the EUV beam to serve as the reference beam, while the pumped region diffracts the EUV probe to from the object beam. The interference of the two beams forms a dynamic hologram that changes as the surface relaxes. By varying the pump-probe delay time, we observe laser-induced surface displacement and subsequent acoustic oscillations in thin metal films. EUV probing in this manner has sub-picometer sensitivity to vertical surface deformation, and is largely free of ambiguities associated with electronic and photoelastic effects that complicate other photoacoustic schemes. In the future, we will extend phase-sensitive detection to study other transient dynamics, such as thermal transport in nanostructures.

8:48AM U23.00005 Resonant mapping of image states on metal surfaces using tunable femtosecond light, KEVIN KNOX, MEHMET YILMAZ, NADER ZAKI, JERRY DADAP, RICHARD OSGOOD, Columbia University, PETER JOHNSON, Brookhaven National Laboratory — We report resonant band mapping using angle-resolved two-photon photoemission measurements of image states on Cu(111) surfaces using a tunable ultrafast femtosecond optical parametric amplifier source. An optical parametrically amplified visible beam is frequency doubled to obtain a tunable fs UV source with photon energies in the 3.6 to 5 eV range. Unoccupied image states are populated by resonant excitation from the occupied sp-like surface state of Cu(111). The image state electrons are then probed by absorption of a second photon of the same energy. Since the surface and image states have different effective masses, resonant excitation occurs at different parallel momenta for each photon energy. By tuning the photon energy we are able to resonantly map both the surface and image state spectra. Our fs laser provides high signal to noise ratio and ultrafast time resolution and the resonant mapping scheme allows for precise measurement of the dispersion and reference planes (the dispersion minimum) of the occupied and excited bands.

1This work was funded by DOE Grant No. DE-FG02-04ER41057

9:00AM U23.00006 Scattering of an Incident Beam by a Magnetic Structure using FDTD, MIGUEL A. ALVAREZ-CABANILLAS, Instituto Politécnico Nacional, CITEDI. — The electromagnetic scattering by a magnetic structure is modeled using finite difference time domain (FDTD). The electromagnetic wave with normal incidence to the magnetic structure has a plane wave front. The incident electric field is chosen perpendicular to the magnetization in the magnetic structure. The electric field is rotated by the magneto-optical Kerr effect (MOKE) and then reflected. This phenomenon is simulated by building the algorithm for FDTD from the Maxwell’s equations, using a Transversal Magnetic distribution of the fields in the numerical mesh. The HKE is introduced in the dielectric constant of the magnetic material. The space of simulation is surrounded by an absorbing boundary condition (ABC). The Perfect Match Layer (PML) was chosen as an ABC with ten layers, enough to reduce the reflected wave. The same size of cells were used in the while mesh. The size of the cells in the space of simulation and the time step were selected in agreement to reduce the numerical instability. The algorithm simulates the correct rotation of the electric field as was predicted by MOKE. The numerical results of the FDTD were compared with the analytic solution in order to verify the algorithm and validate the numerical results.

9:12AM U23.00007 Measurement of the resonance shift in the radar backscattering cross section of thick stainless steel fibers at 35 GHz, SHARHABEEL ALYONES, The Hashinite University, Physics Department, Zarqa 13115, Jordan, CHARLES BRUCE, New Mexico State University, Physics Dept., Las Cruces, NM, 88003 — Measurements of the radar backscattering cross section of stainless steel fibers with low length-to-diameter ratio (thick fibers) had been done at 35 GHz. The intention was to confirm the resonance shift in length predicted by a numerical solution of the general problem of electromagnetic scattering and absorption by finite conducting wires [1]. The numerical methods solves the generalized form of the Pocklington equation, which is valid for both thin and thick fibers. Single particle radar backscattering measurement system was used and the resonance shift had been confirmed for four sets of aspect ratios. The position of the first resonance is shifted to shorter lengths in comparison with the previous analytical solution of the problem by P. Watermann and J. Pedersen [2].


9:24AM U23.00008 ABSTRACT WITHDRAWN —
9:36AM U23.00009 Plasmon Vibrational Delocalization in 1D Disordered Wigner Lattices  
SHIMUL AKHANJEE, JOSEPH RUDNICK, UCLA Dept. of Physics and Astronomy — We explore various aspects of classical 1D Wigner solids in the presence of strong disorder at $T = 0$. Two different realizations of electrostatic randomness are studied: a system of particles with spatially random charge strengths and a system of like charges interacting with an external random potential. In the random potential system we have discovered a novel type of vibrational delocalization transition of the plasma oscillations. Finite size scaling studies of the localization length and inverse participation ratio reveal an Anderson transition from extended to localized eigenmodes at larger eigenfrequencies. Other properties of the eigenmodes are also discussed in the context of this criticality. Additionally, for both models the probability density of particle spacings is examined analytically through the use of probability convolutions within a weak disorder approximation and compared to numerically relaxed ensembles. We find that the statistical configuration of the charges is sensitive to the to the specific type of quenched random distribution.

9:48AM U23.00010 Evidence of Electron-Plasmon Coupling in Single Crystal Bismuth  
RICCARDO TESIO, University of Geneva, Switzerland — We present a detailed optical study via the extended-Drude model analysis of single crystal bismuth using infrared reflectivity and visible-light ellipsometry. The extremely narrow Drude peak and the small value of the screened plasma frequency are consistent with the small carriers density typical for this semimetallic system. The temperature dependence of the optical properties is dominated on one side by the progressive narrowing of the free electron Drude peak and on the other side by the progressive appearance of an absorption peak in the region between the intra-band and inter-band contributions with a consequent change in the frequency dependent scattering rate $\tau^{-1}(\omega)$. We observed that the inflection point $\omega_\tau(\omega)$ corresponding to the increase of $\tau^{-1}(\omega,T)$ closely follows the change of the plasma frequency with temperature according to the relation $\omega_\tau(T) \simeq \omega_p(T)$. This aspect suggests a possible interaction between free electrons and collective modes as already theoretically demonstrated in earlier works. In this scenario we calculated the scattering rate contribution for electron-plasmon interaction starting from the plasmon dispersion relation observing an astonishing good agreement between experimental result and theoretical expectation.

10:00AM U23.00011 Electromagnetic Contribution to Enhanced Raman Scattering from a Metal Nanoshell Dimer  
 Supported by the LDRD program of ORNL and BES program of DOE

10:12AM U23.00012 Convective Atom Transport as a Modifier of Near-Surface Alloy Com- position  
YONG W. KIM, Lehigh University — Thermophysical properties of metallic alloys are manifestly the features of a given material specimen, and, as such, they are dependent on their elemental composition. Some properties are measured at surfaces and others are measured through the bulk as a whole. Complications arise when the elemental composition becomes position dependent within a material specimen. Such occurrences turn out to be common and have been demonstrated by simultaneous measurements of thermal diffusivity and elemental composition by time-resolved spectroscopy of laser-produced plasma (LPP) plume emissions. To further understand the cause, we have investigated the evolution of near-surface composition of Wood’s alloy (composed of 50 W% bismuth, 25W% lead, 12.5 W% tin and 12.5W% cadmium) as a model system under the influence of thermal cycling with, and without, temperature gradient over the specimen. Surface composition modification has been found to take place by accumulation of irregularly spaced gray patches of inhomo- geneous composition on the surface in the presence of temperature gradient. Surface position and depth-resolved determination of elemental composition by LPP spectroscopy has revealed fully 3-D composition structures of the patches. Candidate mechanisms will be discussed.

10:24AM U23.00013 Effects of Zr Doping on the Oxidation of Low-index Crystal Surfaces of Single Crystal beta-Nickel Aluminum  
SERIF URAN, Pittsburg State University, MARCOS GRIMSDITCH, BOYD VEAL, PAUL PAULIKAS, Argonne National Laboratory — Addition of small amount (∼0.1 atm %) of a reactive element (e.g., Y, Zr, Hf) to substrate alloy prior to oxidation is known to improve the oxidation properties (i.e., adherence) of these alloys. This phenomenon is known as the reactive element effect. The purpose of this investigation is to determine the role of reactive element doping during oxidation of a single crystal. It can be argued that absence of grain boundaries in the underlying metal might change or inhibit the improved scale adherence normally produced by doping with a reactive element. By comparing the effects of reactive element doping on the oxidation of different crystallographic faces, we expect to improve our understanding of this still very poorly understood phenomenon. In this study, we have measured scale thickness, composition and residual stress as a function of oxidation temperature for the three principal low-index surfaces (001), (1-10) and (111) of zirconium doped specimen. Systematic differences are observed among different surfaces and the results are compared to those of the undoped crystal.

10:36AM U23.00014 Electronic structure of ultrathin films of Co on Cu(775) stepped surfaces using high-resolution photoemission spectroscopy  
SHANCAI WANG, JERRY DADAP, MEHMET YILMAZ, KEVIN KNOX, NADER ZAKI, RICHARD OSGOOD, Columbia University, TONICA VALLA, PETER JOHNSON, Brookhaven National Laboratory — We perform high-resolution photoemission spectroscopy, using the U13UB UV line at the NSLS, to study the electronic structure of bare and low-coverage Co on Cu(775) stepped surfaces. Despite the relatively wide terrace widths, the bare surface shows clear evidence of umklapps due to the step edges; this behavior is sharpened in the presence of very low Co coverage due to step pinning. We also measure the dispersion for electron emission along and perpendicular to the steps and obtain an exchange splitting energy for the lower Co d-bands at 16 and 25 eV photon energies. The splitting energy reaches a value of as low as ~0.4 eV, which is considerably smaller than that obtained for both Co and Co/Cu(111) surfaces. In addition, the typical widths of the spin states are larger than those obtained for the other surfaces, indicating the increased scattering channels arising from the strong influence of the steps.

1 This work was funded by DOE Grant No. DE-FG02-04ER46157 Mapping the electron response of nanomaterials.

10:48AM U23.00015 Oxidation of Pt (100) surface: Ab initio studies  
EUNJAI KIM, DAVID STUCKE, TAO PANG, Department of Physics, University of Nevada, Las Vegas, NV 89154 — We have performed density-functional calculations to investigate the oxidation process of Pt (100) surface. We carefully examine the previously proposed models and propose a new dissociative model of oxygen molecules on the Pt (100) in this study. Our findings also indicate that one monolayer of oxygen atoms can be covered on Pt (100) surface with 1.09 eV/O2. The role played by oxygen and temperature in the degradation of catalyst will be further discussed in details.

1 This work is supported by the U.S. Department of Energy (DOE) under Award Number DE-FG36-05GO85028.
8:12AM U31.00002 Superfluidity of Grain Boundaries in Solid $^4$He\textsuperscript{1}, NIKOLAY PROKOFIEV, Department of Physics, University of Massachusetts, Amherst, LODE POLLET, Theoretische Physik, ETH Zurich, MASSIMO BONINSEGGI, Department of Physics, University of Massachusetts, MATTHIAS TROYER, ETH Zurich. — We use quantum Monte Carlo methods to demonstrate that the quantum phase transition from normal to superfluid in $^4$He crystals at the melting point is a second-order transition. We find that the transition is not affected by the presence of grain boundaries in the sample. The system displays a rich phase diagram with multiple superfluid phases, including a glassy Bose metal phase and a striped supersolid state.

\textsuperscript{1} NSF Grant No. PHY-0426881.

8:24AM U31.00003 Supersolid is Dirty\textsuperscript{1}, JIANSHENG WU, PHILIP PHILLIPS, University of Illinois — A microscopic model for the supersolid phase in $^4$He is given. On the grain boundary, the motion of atoms is well described by a disordered Bose-Hubbard model. We argue that the clean system is a commensurate Mott insulator but in the presence of disorder, a supersolid state obtains. At work is the disorder-induced closing of the Mott gap. We find that the transition temperature to the supersolid state is an increasing function of disorder as is seen experimentally. In addition, we are able to explain the existence of a superfluid fraction below a characteristic temperature and the pressure dependence of the superfluid fraction. Finally, we also find that a glassy Bose metal phase (BM) is possible and possesses a period shift, though it lacks superflow. This latter observation is useful in explaining the period shift without superflow in hydrogen.

\textsuperscript{1} DMR-0605769

8:36AM U31.00004 Defects and Impurities in Solid $^4$He, KEOLA WIERSCHEM, MARTECH, Dept. of Physics, Florida State University, EFSTRATIOS MANOUSAKIS, MARTECH, Dept. of Physics, Florida State University and University of Athens, Greece — We perform path integral Monte Carlo studies of defects and impurities in solid $^4$He near the low temperature melting transition. The worm algorithm, recently developed for continuum systems, is used to study off-diagonal properties such as the one-body density matrix (OBDM). While this quantity approaches zero exponentially with increasing particle displacement for the "pure" solid, interstitial defects and $^3$He impurities appear to enhance and/or stabilize the OBDM at long distances. This imperfectness in solid helium may lead to the formation of a condensate. These calculations are repeated for two-dimensional solid helium, and compared with results from lattice boson models.

8:48AM U31.00005 Understanding supersolids, MIKLOS GULACSI, ANDRE STOFFEL, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — We model the newly discovered supersolid phase of $^4$He by a hard-core bosonic quantum lattice model in 3 dimension including nearest and next-nearest neighbor interactions. As hard-core Boson exhibit the same algebra as spin-1/2 operators there exists a one-to-one correspondence to the anisotropic Heisenberg model in an external field. To solve this Heisenberg model we used the Tyablikov Green’s function technique and in order to obtain a closed set of equations we used a cumulant decoupling scheme. The obtained Green’s functions have been used to study the properties of the supersolid system such as superfluidity and its phase transition. It was long proposed that vacancies and defects may play a crucial role in the formation of the supersolid phase. Hence we studied the incommensurability which is a measure of the net fraction of vacancies. For the NS phase we re-obtained the well-known thermal activation theory. However, the incommensurability in the SS displays a rather different behavior, which also suggests that the NS to SS transition is a commensurate-incommensurate transition.

9:00AM U31.00006 Field Induced Supersolid Phase in Spin-One Heisenberg Models, PINAKI SENGUPTA, CRISTIAN BATISTA, Los Alamos National Laboratory — We use quantum Monte Carlo methods to demonstrate that the quantum phase diagram of the $S=1$ Heisenberg model with uniaxial anisotropy contains an extended supersolid phase. We also show that this Hamiltonian is a particular case of a more general and ubiquitous model that describes the low energy spectrum of a class of isotropic and frustrated spin systems. This crucial result provides the required guidance for finding experimental realizations of a spin supersolid state.

9:12AM U31.00007 A striped supersolid phase in bosons on the triangular lattice, ROGER MELKO, Oak Ridge National Laboratory — Using large-scale quantum Monte Carlo simulations, we explore the ground-state phase diagram of bosons hopping on a triangular lattice with nearest (V) and next-nearest (V’) neighbor repulsive interactions. In the limit where V=0 but V’ is large, we find an example of an unusual striped supersolid state that is stable at 1/2-filling. We discuss the peculiar properties of this phase, as well as the phase transitions out of it into the neighboring superfluid and Mott phases.

9:24AM U31.00008 Theory of Small Para-Hydrogen Clusters: Magic Numbers and Superfluid Sizes\textsuperscript{1}, SAAD KHAIROLLAH, Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA, MIKHAIL SEVRYUK, Institute of Energy Problems of Chemical Physics RAS, Moscow 119334, Russia, DAVID CEPERLEY, NCSA and Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA, PETER TOENNIES, Max-Planck-Institut fur Dynamik und Selbstorganisation, D-37073 Gottingen, Germany — We apply the Path Integral Monte Carlo method to study the low temperature structures and superfluidity of parahydrogen clusters with up to 40 molecules. We find an enhanced stability at certain magic cluster sizes and sharp jumps in superfluidity for specific cluster sizes (V > 2n). Superfluidity is largely localized on the surface and coexists with clusters with solid-like core.

\textsuperscript{1} US DOE (DEFG02-91ER45439), NSF (DMR-03 25939 ITR) and NASA (NAG-8-1760).

Thursday, March 8, 2007 8:00AM - 10:36AM — Session U31 DCMP: Supersolids Theory Colorado Convention Center 401
9:36AM U31.00009 Computer simulations of helium-solvated ions: solid-like versus liquid-like defect structures, STEFANO PAOLINI, FRANCESCO ANCILOTTO, FLAVIO TOIGO, INFN-DEMODRITOS National Simulation Center (Trieste, Italy) and Physics Department “G. Galilei”, University of Padova (Italy). The local order around several alkali (Li$^+$ and Na$^+$) and alkali-earth (Be$^+$, Mg$^+$ and Ca$^+$) ions in $^4$He clusters has been studied using ground-state path integral Monte Carlo simulations. We apply a criterion based on multipole dynamical correlations to discriminate between solid-like versus liquid-like behavior of the He solvent surrounding the impurity-ion. In agreement with existing experimental measurements in bulk helium, our findings suggest that Be$^+$ produces a solid- (“snowball”)-like structure, similarly to alkali ions and in contrast to heavier alkali-earth ones, for which a liquid-like environment is predicted.

9:48AM U31.00010 The BCS-BEC crossover in density in GaAs heterostructures for bilayers of electrons and holes with mismatched densities, DAVID NEILSON, PIERBIAGIO PIERI, GIACARLO STRINATI, University of Camerino — We have investigated excitonic superfluidity in electron-hole bilayers in GaAs at low temperatures. We analyze the crossover from the BCS limit of overlapping pairs (high carrier density) to the BEC limit of non-overlapping tightly-bound pairs (low carrier density) by independently varying the densities of the electrons and holes. The different electron and hole effective masses in GaAs causes the phase diagram to depend strongly on the direction of the density imbalance. We can identify the crossover region between the BCS and BEC regimes in the phase diagram, and we find the richest variety of phases in this crossover region. We propose detection of a jump in the electron and hole chemical potentials across zero-density imbalance as the criterion for the occurrence of superfluidity. We make a comment on the relation of our results to density and mass imbalances in ultracold Fermi atoms.

10:00AM U31.00011 ABSTRACT HAS BEEN MOVED TO S31.00014 —

10:12AM U31.00012 Possible role of $^3$He impurities in solid $^4$He, EFSTRATIOS MANOUSAKIS, Department of Physics, Florida State University, USA, and Department of Physics, University of Athens, Greece. We use a quantum lattice gas model to describe the essential aspects of the motion of $^4$He atoms and of a $^3$He impurity in solid $^4$He. We find that $^3$He impurities promote $^4$He atoms to interstitial sites and this can turn the bosonic quantum crystal into a metastable supersolid. It is suggested that $^3$He impurity atoms, which produce the interstitial $^4$He atoms, might have been reabsorbed by pure $^4$He solid formed during the first stage of a multi-stage solid $^4$He nucleation process. While we use the “spin”-wave approximation and low dimensional lattices to illustrate some of the ideas, we argue that the conclusions drawn from these studies may be valid for the real system.

10:24AM U31.00013 Magnetothermoelectric response at a superfluid–Mott insulator transition, MIRACULOUS BHASEEN, Oxford University, ANDREW GREEN, University of St Andrews, SHIVAJI SONDHI, Princeton University — We present recent results on the finite temperature magnetothermoelectric response in the vicinity of a superfluid–Mott insulator quantum phase transition [cond-mat/0610887]. We focus on the particle-hole symmetric transitions of the Bose–Hubbard model, and combine Lorentz invariance arguments with entropy drift and quantum Boltzmann calculations. Depending on the ratio of the applied fields, the model displays distinct regimes of behavior. We discuss how a non-vanishing thermoelectric tensor and a finite thermal conductivity are supported in this quantum critical regime.

Thursday, March 8, 2007 8:00AM - 11:00AM – Session U42 DCMP: Nitrides, Carbides, Oxides: Surfaces and Properties  Colorado Convention Center 505

8:00AM U42.00001 Electronic structure of nitride surfaces, CHRIS G. VAN DE WALLE, DAVID SEGEV, ANDERSON JANOTTI, Materials Department, University of California, Santa Barbara, California 93106, USA. Knowledge of surface reconstructions and the corresponding surface electronic structure is important to control growth, since Fermi-level pinning can affect defect creation and incorporation. In addition, surface states can play an important role in devices, for instance in high-electron mobility transistors where the surface acts as a source of electrons for the channel. In the case of overlapping pairs (high carrier density) to the BEC limit of non-overlapping tightly-bound pairs (low carrier density) by independently varying the densities of the electrons and holes. The different electron and hole effective masses in GaAs causes the phase diagram to depend strongly on the direction of the density imbalance. We can identify the crossover region between the BCS and BEC regimes in the phase diagram, and we find the richest variety of phases in this crossover region. We propose detection of a jump in the electron and hole chemical potentials across zero-density imbalance as the criterion for the occurrence of superfluidity. We make a comment on the relation of our results to density and mass imbalances in ultracold Fermi atoms.

8:12AM U42.00002 Electronic structures and work functions of InN(0001) films, JUNG-HWAN SONG, ARTHUR J. FREEMAN, Northwestern U. — InN films have attracted great attention with its recently discovered band gap, 0.7eV, and evidence for p-type doping. We have studied theoretically the electronic structures, surfaces, and work functions of InN films using the highly precise FLAPW method. The passivation with pseudo-hydrogen has also been applied to the surfaces of InN(0001) films for comparison with the electronic structure of the ideal InN(0001) films. We compare the work functions of InN films with other wurtzite materials such as ZnO, GaN, and AlN, which we have also calculated. We discuss the mechanism of the structural transition with layer thickness for the very thin InN(0001) films, for which we have found that the ideal InN(0001) films of the wurtzite structure, up to 4 bilayers, optimize to the graphite-like structure. We then discuss the relationship between the dipoles and the surfaces (work functions) of the InN(0001) films, and the possibilities of their p-type doping.

1Supported by NSF (through its MRSEC program at N.U.) and DOE.
9:00AM U42.00006 Growth and Structure of ZrSiN Thin Films, ROBERT LAD, XUEFEI ZHANG, University of Maine — A series of Zr$_{1-x}$Si$_x$N thin films were grown on r-plane sapphire substrates using rf magnetron co-sputtering of Zr and Si targets in a N$_2$/Ar plasma. The films were grown at 200°C and post-deposition annealed to 900°C in vacuum. Pure ZrN grows with high quality (100) epitaxy on r-sapphire as demonstrated by x-ray diffraction reflectivity and pole figure analysis. When small amounts of Si are added into the lattice, the films become strained as evidenced by a continual increase in the lattice parameter (up to a 6% for x=0.12) and become polycrystalline. Higher amounts of Si cause the structure to become amorphous and the films become much rougher. X-ray photoelectron spectroscopy measurements show large shape changes in the N and Zr core levels as the alloy composition changes, whereas the Si peaks exhibit negligible change. UV-visible optical absorption measurements show a direct correlation between the location of the absorption edge and Zr-Si ratio.

9:12AM U42.00007 Passivation of 4H-SiC Silicon surface, G. PENNINGTON, University of Maryland, College Park, C. ASHMAN, High Performance Technologies Inc., A. LELIS, U.S. Army Research Laboratory, N. GOLDMAN, UNIVERSITY OF MARYLAND ELECTRICAL AND COMPUTER ENGINEERING DEPT. COLLABORATION, DOD HPCMP PET PROGRAM COLLABORATION, U.S. ARMY RESEARCH LABORATORY, ADELPHI, MD. COLLABORATION — The material properties of the silicon carbide (SiC) 4H polytype are ideally suited for use in metal-oxide-semiconductor (MOS) devices. Recent advances in laser etching and other wet etching methods have made it possible to produce surfaces of good quality. However, the surface passivation of these surfaces is a critical issue for device performance. In this work, we have investigated the passivation of 4H-SiC surfaces using a combination of X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FTIR), and atomic force microscopy (AFM). We have found that the use of a thin layer of ZnO on the surface can significantly improve the passivation properties of the 4H-SiC surface. This work is supported by the U.S. Dept. of Energy contract DE-AC02-06CH11357.

9:24AM U42.00003 HREELs, AES, and LEED of InN(000-1): Surface structure and electron accumulation, RUDRA BHATTA, BRIAN THOMS, MUSTAFA ALEVLI, NIKOLAUS DIETZ, Georgia State University — InN layers grown by high pressure chemical vapor deposition (HPCVD) have been studied using several surface sensitive techniques. Following argon sputtering and atomic hydrogen cleaning (AH), Auger electron spectroscopy showed that surface contaminants had been removed and a 1x1 hexagonal low energy electron diffraction pattern demonstrated that the InN surface was well ordered. HREEL spectra of the atomic hydrogen cleaned layer show a Fuchs-Kliewer surface phonon at 560 cm$^{-1}$ and adsorbate loss peaks at 3260 and 870 cm$^{-1}$ assigned to N-H stretching and bending vibrations, respectively. These assignments are confirmed by isotopic shifts using deuterium. No surface In-H vibrations are observed indicating N-H termination of the surface and the film is N-polar. HREEL spectra also showed a broad loss features due to conduction band plasmon excitations. The plasmon excitation shifted to higher energy as the incident electron energy (and therefore the penetration depth) was decreased. This shift indicates that the surface has a higher plasma frequency than bulk of the InN layer, which in turn indicates the presence of a surface electron accumulation layer.

8:36AM U42.00004 In-situ X-ray Studies of MOCVD Growth of InN, FAN JIANG, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, A. MUNKHOLM, C.D. DIMITROPOULOS, Philips Lumileds Lighting Company, San Jose, CA 95131, R.-V. WANG, S.K. STREIFFER, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439, G.B. STEPHENSON, P.H. FUOSS, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, K. LATIFI, CAROL THOMPSON, Physics Department, Northern Illinois University, DeKalb, IL 60115 — One of the fundamental issues in the continued development of III-nitride semiconductor alloys is to understand incorporation of indium. Our approach is to use real-time x-ray scattering and fluorescence as in situ probes during growth by MOCVD. We observe the equilibrium condensation boundaries for elemental In and InN as a function of temperature and trimethylindium supply, which allow us to determine the effective activities of In and N at the surface. We find that the partial pressures of both hydrogen and ammonia in the ambient have strong effects on the activities. We also observe strong effects of the substrate on condensation, including an oscillatory regime, indicating that surface reactions are important. Work supported by the U.S. Dept. of Energy contract DE-AC02-06CH11357.

8:48AM U42.00005 Atomic and Electronic Structures of Oxygen on the $\beta$-$\text{Si}_3\text{N}_4$ (10$\overline{1}$0) Surface, WERONIKA WALKOSZ, JUAN C. IDROBO, SERDAR OGUT, University of Illinois at Chicago — The desirable mechanical and physical properties of Si$_3$N$_4$ ceramics make them attractive for high temperature applications. Doping Si$_3$N$_4$ with rare-earths has long been known to overcome this limitation creating a tough material. Precise information about the microscopic origin of this empirical observation has, however, been lacking for many years. In this study, we present ab initio calculations for the structural stability of $\beta$-$\text{Si}_3\text{N}_4$ (10$\overline{1}$0) surfaces in the presence of different oxygen concentrations. Two different (10$\overline{1}$0) surface terminations, the “open ring” and the “half surface” are investigated in detail using an asymmetric slab. We find that the Si-O bond plays the most important role in the structural stability and passivation of the surface. The theoretical results are analyzed in connection with recent electron microscopy studies on the interface.

1Work supported by NSF Grant No. DMR-0605964
9:36AM U42.00009 Role of neutral impurity scattering in the analysis of Hall data from ZnO

9:48AM U42.00010 Direct observation of zinc vacancies and oxygen vacancies in an electron-irradiated ZnO crystal.

10:00AM U42.00011 Tunable UV-Luminescent MgZnO Nanoalloys

10:12AM U42.00012 Stability, Electronic and Optical Properties of In$_n$O$_3$($\text{ZnO})_n$ Alloys

10:24AM U42.00013 Carrier Dynamics and Emission Efficiency in Sulfur-doped ZnO Powders

10:36AM U42.00014 Origin of high-density two-dimensional electron gas in ZnO/ZnMgO heterostructures.

10:48AM U42.00015 Anisotropic thermal expansion in wurtzite materials: an ab-initio calculation for ZnO.
8:00AM U43.00001 Γ-phonons in ZnSe(C2H8N2)1/2 and ZnTe(C2H8N2)1/2 hybrid materials, IVAN NAUMOV, HUAXIANG FU, Department of Physics, University of Arkansas — Artificially synthesized organic/inorganic hybrid materials with a semiconductor component are of growing interest due to potential applications in flexible microelectronics. Among them, hybrid ZnSe(C2H8N2)1/2 and ZnTe(C2H8N2)1/2 are two examples capable of tuning electronic and optical properties on a wide range. Engineering of these materials is difficult without deeper understanding of their fundamental physical characteristics, including electronic band structure and phonon spectra. Recent experimental investigations [1] performed on ZnSe(C2H8N2)1/2 samples and showed multiple sharp phonon modes in frequencies very different from the LO(T) phonon of the binary semiconductor ZnTe. Motivated by these results, we have performed density-functional calculations of the Γ phonon modes for both α- and β-phases of ZnSe(C2H8N2)1/2 and ZnTe(C2H8N2)1/2. We found, in particular, that light hydrogen atoms not only define the high frequency phonon (1500–3000 cm⁻¹), but also dominate in some low frequency modes in the region of 100-150 cm⁻¹ where they move mostly perpendicular to the superlattice stacking direction. Based on symmetry of the materials, the Raman modes at the Γ point are identified.


8:12AM U43.00002 The Magnetic-Field Dependent Phonon-Like FIR Absorption in Modulation Doped CdMnTe/CdMgTe quantum Well Structures, LI-CHUN TUNG, National High Magnetic Field Laboratory at Florida State University, GRZEGORZ KARCZEWSKI, Institute of Physics, Polish Academy of Science, YONG-JIE WANG, National High Magnetic Field Laboratory at Florida State University — Spin-dependent phonon had been reported in several magnetic semiconductors. This unique phonon mode is resulted from an ion-position dependent spin Hamiltonian. This mode can be either infrared or Raman active. However, such modes were never observed in the diluted magnetic semiconductors.

8:24AM U43.00003 ABSTRACT WITHDRAWN —

8:36AM U43.00004 Investigation of the influence of the magnetic field of different orientations on exciton states in structures with shallow quantum wells, YURI KHAVIN, MIKHAIL SKORIKOV, NIKOLAI SIBELEIDN, VITALIY TSVEKOV, P.N. Lebedev Physical Institute, Russian Academy of Sciences, Moscow, Russia — Photoluminescence (PL) and photoluminescence excitation (PLE) spectra of GaAs/Al0.5Ga0.5As structures with two tunneling-coupled quantum wells (QWs) 3 and 4 nm wide and structures with tunneling-isolated QWs of the same width were investigated at liquid helium temperatures in parallel and perpendicular magnetic fields up to 14.6T. It was shown that the parallel magnetic field strongly suppresses tunneling coupling in the structure with coupled QWs, and its PLE spectrum in a strong field becomes similar to the PLE spectrum of the structure with isolated QWs. At the same time, excitonic components of the PL spectrum do not undergo such substantial changes. It was also shown that both parallel and perpendicular field substantially affect the intensity of the trion PL line in both structures, but the influence of the parallel field is much stronger than it is for the perpendicular field.

8:48AM U43.00005 Photoluminescence Studies of Type-I and Type-II In0.27Ga0.73Sb/In0.8As/In0.53Sb Multiple Quantum Well Heterostructures Grown by MBE, E.R. GLASER, R. MAGNO, B.V. SHAÑABROOK, J.G. TISCHLER, Naval Research Lab, NAVAL RESEARCH LAB TEAM — Heterojunction bipolar transistors (HBTs) with lattice constant near 6.2Å using the InAs/AlSb/GaSb family of semiconductors are of interest based on their promise for high-speed operation with low power dissipation. A unique aspect of these materials is the ability to engineer the bandgap energies and the conduction band offsets at the emitter/base and base/collector heterointerfaces by varying the In/Al and Al/Sb ratios. In this work, low-temperature PL was performed on a set of In0.27Ga0.73Sb/In0.8As/In0.53Sb MQW heterostructures to provide a measure of the conduction band offsets (ΔCB) that are a critical design parameter for the HBTs. Excitation power studies revealed evidence for strong recombination at 0.56 eV within the InGaSb layer of the MQW structure with x,y = 0.52,0.25 and, thus, confirmed the type-I band alignment. In contrast, weaker PL bands at energies close to 0.4 eV were observed with exhibited strong shifts with increasing excitation power density were found from the nominally type-II MQW samples with x,y = 0.67,0.39 and 0.69,0.41. Neglecting small corrections (~15 meV) due to the electron and hole confinement energies, we estimate ΔCB of ~ 120-150 meV in these Type-II structures.

9:00AM U43.00006 Temperature and Pump Pulse Dependence of Superfluorescence from InGaAs/GaAs Multiple Quantum Well in High Magnetic Fields, XIAOMING WANG, YOUNG-DAHLL JHO, JINHO LEE, DAVID REITZE, University of Florida, JUNICHIRO KONO, Rice University, ALEXEY BELYANIN, VITALY KOCHAROVSKY, Texas A&M University, GLENN SOLOMON, Stanford University, XING WEI, STEPHEN MCGILL, NHMFL — Using intense near-IR ultrashort pulse laser excitation, we investigated the characteristics of cooperative emission (superfluorescence) from dense electron hole magneto-plasmas in InGaAs/GaAs MQW in high magnetic fields as a function of temperature and excitation pulsewidth. We find strong narrow line emissions from 0-0 and 1-1 Landau levels (LLs), with thresholds depending on magnetic field and temperature. Varying the excitation pulsewidth (180 fs – 60 ps) and fluence (0.1 – 1 mJ/cm²), we observe qualitative changes in the emission strengths from different LLs. The strong emissions from 0-0 and 1-1 LL excited with short and long pulses are obviously different. Mechanisms of the temperature and excitation pulse width effect on the strong emission are presented.

1Supported by the NSF through grant DMR-0325499 and by the NHMFL through an IHRP grant.
9:12AM U43.00007 Interface roughness scattering in p-Si/SiGe asymmetric quantum wells .
MARCO CALIFANO, N.Q. VINH, P.J. PHILLIPS, Z. IKONIC, R.W. KELSALL, P. HARRISON, C.R. PIDGEON, B.N. MURDIN, D.J. PAUL, P. TOWNSEND, J. ZHANG, I.M. ROSS, A.G. CULLIS, School of Electronic and Electrical Engineering, University of Leeds, U.K. — Of paramount importance in the design of a quantum cascade laser is the ability to engineer carrier lifetimes. These can be strongly influenced by the quality of the interfaces: fluctuations in the well width result in local fluctuations of the carriers’ confining potential, which act as a scattering potential. We report the direct determination of non-radiative lifetimes in Si/SiGe asymmetric quantum wells designed to access spatially indirect intervalley transitions between heavy-hole states, at photon energies below the optical phonon energy. We show both experimentally and theoretically that, for the interface quality currently achievable experimentally interface roughness will dominate all other scattering processes up to about 200 K. By comparing our results obtained for two different structures we deduce that in this regime both barrier and well widths play an important role in the determination of the carrier lifetime. Comparison with recent data for III-V multiple quantum wells leads us to the conclusion that the dominant role of interface roughness scattering at low temperature found here is a general feature of a wide range of semiconductor heterostructures not limited to IV-IV materials.

9:24AM U43.00008 Localized charged magnetoexcitons in 2D systems1 .
DIANA COSMA, ALEXANDER TODD, ALEXANDER DZYUBENKO, CSU Bakersfield, Bakersfield, CA93311, ANDREY SIVACHENKO, Ariadne Genomics Inc., Rockville, MD 20850 — We performed a detailed theoretical study of localization of spin-singlet X+ and spin-triplet X− negatively charged excitons on isolated charged donors D+ located at various distances L from the heteroboundary of a Quantum Well (QW). Our results show that the parent bright singlet state X+ remains always bound. In contrast, the dark X− and bright X+ triplet states survive only for sufficiently large distances L to the donor ion D+. In the presence of a D+ the dark triplet acquires finite oscillator strengths. We also found several new bound X− states, some of which have surprisingly large oscillator strengths. We showed that shake-up processes are strictly prohibited in magneto-polaritoumnescence of free charged excitons and only become allowed in the presence of a D+ or other symmetry-breaking mechanisms. Our results show that the magneto-PL peaks of free and donor bound charged excitons may exhibit very similar features while the shake-up processes in PL are symmetry-breaking signatures.

1Supported in part by DMR-0203560 and DMR-0224225, and by a College Award of Cottrell Research Corporation.

9:36AM U43.00009 Effect of disorder on the lifetime of interface polaritons .
IGOR SMOLYARENKO, Brunel University, CELESTINO CREATORE, ALEXEI IVANOV, Cardiff University — We study the effects of weak disorder on the lifetime of interface polaritons in quantum wells (QWs) associated with in-plane free QW excitons. In ideal quantum wells, the interface light is evanescent, i.e., it is localized in the z direction (QW growth direction) and is thus invisible at macroscopic distances from the QD plane. However, randomness in the structure of QWs leads to finite radiative lifetimes of the interface light modes which makes them “visible” in time-resolved light scattering experiments. We study the distribution of the delay times for scattering of bulk photons off the two-dimensional interface layer at finite incidence angle. While the bulk of the distribution corresponds to the usual threshold effect, the tail of the distribution at long delay times is governed by the quasi-resonant long-lived interface light modes which are essentially the disorder-degraded remnants of the evanescent waves in ideal QWs. These modes are analogous in some ways to the anomalously localised states in two-dimensional disordered electronic systems. Time-resolved spectroscopy of weakly disordered QWs is thus shown to be an effective tool for probing the “hidden” optics of the interface polaritons.

9:48AM U43.00010 Generic Theory of Surface Plasmon Polaritons at Active or Passive Metal-Dielectric Interfaces .
DENTCHO GENOV, MURALIDHAR AMBATI, XIANG ZHANG, University of California at Berkeley — In this work we propose a simple analytical approach to study the excitation of surface plasmon polaritons (SPP) at the interfaces between metals and passive or active media. Explicit relationships are derived for both SP dispersion and propagation length. The analytical theory matches the exact numerical calculations for a wide range of excitation frequencies and metal slab thicknesses. Scaling relationships for the critical gain required to achieve infinite propagation length are derived for the symmetric and antisymmetric SPP modes. A specific multiple quantum well (MQW) system is identified as an effective media for prospective experimental studies of SP amplification and enhanced propagation.

10:00AM U43.00011 Nonequilibrium Green’s function modelling of quantum well solar cells .
URS AEBERHARD, RUDOLF H. MORF. Condensed Matter Theory, Paul Scherrer Institut — We present a microscopic model of the photocurrent in GaAs – AlGaAs quantum well solar cells (QWSC), based on the nonequilibrium Green’s function formalism (NEGF) for a multiband tight binding Hamiltonian. The quantum kinetic equations of motion are selfconsistently coupled to Poisson’s equation. Relaxation and broadening mechanisms are considered by the inclusion of acoustic and optical electron-phonon interaction in a self consistent Born approximation of the scattering selfenergies. The model is applied to different multi-quantum well systems to investigate the role of device geometry and coupling between the wells.

10:12AM U43.00012 Optical and Electronic Properties of Electrochemically Active Perylene Tetracarboxylic Diamide Molecules .
NAZANIN DAVANI, Department of Chemical Engineering, Stanford University, KEN SHIMIZU, Department of Material Science and Engineering, Stanford University, MICHAEL PREINER, Department of Applied physics, Stanford University, NICHOLAS MELOSH, Department of Material Science and Engineering, Stanford University, MELOSH GROUP TEAM — Perylene tetracarboxylic diamide (PTCDI) molecules form a unique class of n-type semiconductors with high thermal and photo stability. Understanding the electronic properties of these molecules in nanoscale systems may lead to novel applications in various molecular electronics devices. Using optical spectroscopy, we analyzed the optical and electronic properties of electrochemically active TE-PTCDI molecules self-assembled on gold electrodes. Surface Plasmon Resonance Spectroscopy is used to detect the refractive index of the monolayer. Cyclic voltammetry and SPR measurements are performed simultaneously to probe changes in reflectivity as the molecule undergoes redox reactions. In addition, the TE-PTCDI molecule is used in fabricating metal-insulating monolayer-metal devices using Polymer Assisted Lift Off (PALO) technique. The influence of the top metal contact on molecular properties will be discussed.

10:24AM U43.00013 Photoconductivity of Yttrium Neodymium Gadolinium Oxalate Crystals1 .
SOOSY KURYAN, ROSALIN ABRAHAM, JAYAKUMARI ISAC, SOOSY KURYAN TEAM — Crystals are pillars of modern technology. Yttrium Neodymium Gadolinium oxalate (YNdGaOx) crystals were grown by gel method by the diffusion of Yttrium Chloride, Neodymium Chloride, and Gadolinium Chloride into the set gel containing Oxalic acid. Silica gel method is capable of yielding crystals of high optical perfection and wide morphology. The growing crystals are held in the gel medium in a strain free manner and at the same time nucleation and super saturation are well controlled. Photo conductivity studies of these crystals revealed negative photoconductivity nature. The photocurrent is found to be less than the dark current at every applied electric field. Rare Earth compounds are known for their interesting electric, magnetic and luminescent properties. Recent investigations on the fluorescence of some rare earth oxalates suggest their potentiality for their optical applications. Rare Earth oxalates evoked greater attention because of their ionic conduction.

1University Grant Commission.
10:36AM U43.00014 Plasmon dispersion and Coulomb drag in low-density electron bi-layers¹
S. M. BADALYAN, Yerevan State University, C. S. KIM, Chonnam National University, G. VIGNALE, University of Missouri, C. SENATORE, University of Trieste — We investigate the effect of exchange and correlation (xc) on the plasmon spectrum and the Coulomb drag between spatially separated low-density two-dimensional electron layers. We adopt a new approach, which employs dynamic xc kernels in the calculation of the bi-layer plasmon spectra and of the plasmon-mediated drag, and static many-body local field factors in the calculation of the particle-hole contribution to the drag. We observe that both optical and acoustical plasmon modes are strongly affected by xc corrections and shift in opposite directions with decreasing density. This is in stark contrast with the tendency observed within the random phase approximation (RPA). We find that the introduction of xc corrections results in a significant enhancement of the transrelativity and qualitative changes in its temperature dependence. In particular, the large high-temperature plasmon peak that is present in the RPA is found to disappear when the xc corrections are included. Our numerical results are in good agreement with the results of recent experiments by M. Kellogg et al., Solid State Commun. 123, 515 (2002).

¹Work supported DAAD, KOSEF Grant No. R05-2003-000-11432-0, and NSF Grant No. DMR-0313681

10:48AM U43.00015 Surface Plasmon Polaritons on Concentric Cylindrical Shells, JAKUB PRITZ, LILIA WOODS, University of South Florida — A theoretical investigation of electromagnetic plasmon modes for multilayered concentric cylindrical shells in the absence of an applied magnetic field is presented. These plasmon excitations in such multiple interface configurations are characterized by the electromagnetic fields. To obtain the dispersion relation for the modes, the Maxwell equations with appropriate boundary conditions are solved numerically. We study the conditions for existence of radiative and nonradiative modes. The effects of varying the different shells radii, their thicknesses and dielectric response functions are also investigated. The physical importance of the different plasmon modes is also discussed.

Thursday, March 8, 2007 11:15AM - 2:15PM
Session V1 DCMP: New Developments in Supersolids
Colorado Convention Center Four Seasons 2-3

11:15AM V1.00001 Squeezing superfluid from a stone: Coupling superfluidity and elasticity in a supersolid, ALAN DORSEY, University of Florida — Superfluidity—the ability of liquid $^4$He, when cooled below 2.176 K, to flow without resistance through narrow pores—has long served as a paradigm for the phenomenon of “off-diagonal long-range order” (ODLRO) in quantum liquids and superconductors. Supersolidity—the coexistence of ODLRO with the crystalline order of a solid—was proposed theoretically over 35 years ago as an even more exotic phase of solid $^4$He, but it has eluded detection. Recently, Kim and Chan [1,2] have reported an anomalous decoupling transition of solid $^4$He in a torsional oscillator measurement, and interpret their results as evidence for non-classical rotational inertia and a possible supersolid phase of $^4$He. In this talk I will give brief historical review of the theory of and experimental searches for supersolidity. I will then discuss a phenomenological Landau theory of the normal solid to supersolid (NS-SS) transition in which superfluidity is coupled to the elasticity of the crystalline $^4$He lattice, and underscore the implications of this theory for experimental searches for supersolidity [3]. I will also discuss a hydrodynamic model for supersolids, in which the additional broken gauge symmetry in the supersolid phase produces a collective mode that is analogous to second sound in superfluid helium.


11:51AM V1.00002 Elimination of the Supersolid State Through Crystal Annealing¹, JOHN REPPY, Cornell University — We have employed the torsional oscillator technique in the study of the supersolid state of solid $^4$He. We find that the supersolid state is not a universal property of solid helium, but in certain cases can be reduced or even eliminated through an annealing of the sample. We have also studied the supersolid in a number of cells with differing geometries, including cylindrical, cubic, and annular geometries, in an attempt to examine the possible influence of geometry on the stability of the supersolid state.

¹Work supported by the National Science Foundation through Grant DMR-0605864

12:27PM V1.00003 Superfluidity of grain boundaries and supersolid behavior, SEBASTIEN BALIBAR, ENS-Paris (France) — We have found that, at the liquid-solid equilibrium pressure $P_m$, supersolid behavior is due to the superfluidity of grain boundaries in solid helium [1]. After describing this experiment and reviewing some of the related theoretical work [2], we discuss the possibility that, at larger pressure ($P > P_m$), grain boundaries could also explain the supersolid behavior which was observed with torsional oscillators [3-6].


1:03PM V1.00004 Supersolids? , DAVID HUSE, Princeton University — A brief, biased and selective review will be given of various theoretical and experimental results (recent and not so recent) addressing questions of supersolidity and related properties of quantum solids, especially helium.

1:39PM V1.00005 Measurements on the melting curve of $^4$He down to 10 mK, HARRY ALLES, Low Temperature Laboratory/Helsinki University of Technology — Recent discovery of a nonclassical rotational inertia in solid $^4$He below about 0.2 K by Kim and Chan has initiated an intensive study on the properties of solid $^4$He. As Kim and Chan have interpreted their observation as the evidence of supersolid behavior, we have decided to measure very accurately the melting curve of $^4$He down to 10 mK. After about 0.5 microbar with $^4$He crystals which had various concentration of defects. All our samples showed only the expected $T^3$ dependence due to phonons without any sign of the supersolid transition in the temperature range of 80...400 mK. Below 80 mK we observed a small deviation from $T^3$ dependence which, however, cannot be attributed to the supersolid transition because our recent measurements with the cell containing liquid sample only suggest that this deviation is by the temperature variation of properties of BeCu membrane of our capacitive pressure gauge. In addition to our published data with $^4$He of natural purity [Phys. Rev. Lett. 97, 165302 (2006)] we also report our recent measurements of the melting curve with ultra pure $^4$He (0.3 ppb of $^4$He impurities). In these measurements we followed optically the shape of the sample crystals which had very good quality.
The images reveal the location of the quantum dots along the wire and the tip voltage can tune their charge state. movable gate to change the induced charge on a single dot in a spatially dependent way, down to zero electrons. We have also imaged homogeneous InAs quantum dot; the rings correspond to Coulomb-blockade oscillations of the quantum dot. In this way the tip locates the quantum dot and can be used as a field-effect transistors, where issues related to lateral and vertical processing of nanowires will be addressed.

Kinetic measurements during the vapor-liquid-solid growth of Si and Ge nanowires, SUNEEL KODAMBAKA, IBM — Growth of nanowires using vapour-liquid-solid (VLS) process has been successfully demonstrated over the past 40 years, but the exact mechanisms are not well understood. In this talk, we will present in situ transmission electron microscopy studies of Si and Ge nanowire growth kinetics as a means to develop a fundamental understanding of the mechanisms governing their shape and structure. From the images of the wires, collected at video rates as a function of growth pressure, temperature, and gas environment, we identify several novel aspects of wire growth: Ostwald ripening of catalyst droplets on top of the wires, effect of oxygen on Si wire morphology, and VLS growth of Ge wires at temperatures below the bulk Au-Ge alloy eutectic temperature. We will consider the generality and applicability of these results for the growth of nanowires of other materials.

Spin properties of strongly interacting quantum wires, JULIA S. MEYER, The Ohio State University — A number of recent experiments on quantum wires report deviations from perfect conductance quantization at low densities. These conductance anomalies manifest themselves as quasi-plateaus in the conductance as a function of gate voltage at about 0.5 to 0.7 of the conductance quantum $G_0 = 2e^2/h$, depending on the device. Most commonly the experimental findings are attributed to non-trivial spin properties of quantum wires. In particular, spontaneous spin polarization of the ground state has been proposed as a possible origin of the conductance anomalies. The issue has generated a lot of interest in the community as this interpretation is in apparent contradiction with the Lieb-Mattis theorem, which forbids spontaneous spin polarization in one dimension. However, the spin properties may change dramatically when the system becomes quasi-one-dimensional. We show [1] that sufficiently strong interactions between electrons induce deviations from the strictly one-dimensional geometry and indeed give rise to a ferromagnetic ground state in a certain range of electron densities. A novel phase with more complicated spin interactions generated by four-particle ring exchanges is identified at higher densities. [1] A.D. Klimonos, J.S. Meyer, and K.A. Matveev, Europhys. Lett. 74, 679 (2006).

Mesoscopic Josephson Junctions Employing Ge/Si Core/Shell Nanowires, ANDY VIDAN, MIT Lincoln Laboratory — Semiconductor nanowires are finding increased importance in nanoelectronics due to their controlled growth and reduced dimensions. Band structure engineering of heterostructure nanowires is proving to be instrumental in creating low-dimensional carrier gases with enhanced mobility, low scattering and reproducible contacts. We present low temperature transport measurements of one-dimensional hole gases formed in (undoped) germanium/silicon (Ge/Si) core/shell heterostructure nanowires. The Ge core diameter of the nanowires is 15 nm with a 2 nm Si shell. The length of the nanowire between the contacts is typically 150 nm. Transparent contacts to the nanowires allow observation of transport through one-dimensional subbands arising from radial confinement. When connected to superconducting aluminum leads, a dissipationless supercurrent flows through the semiconductor nanowire due to proximity-induced superconductivity. By using a Au top gate, which modulates the carrier density of the nanowire and the number of one-dimensional subbands populated, the critical current of these mesoscopic Josephson junctions can be tuned from zero to greater than 100 nA. Resonant multiple Andreev reflections in the superconductor-nanowire-superconductor system is also observed. Finally, we investigate the interplay between one-dimensional quantum confinement and superconductivity.

Mesoscopic Josephson Junctions Employing Ge/Si Core/Shell Nanowires

This work was performed in collaboration with Jie Xiang, Charles M. Lieber, M. Tinkham, and R.M. Westervelt at Harvard University.

Imaging Few-Electron Quantum Dots in InAs/InP Nanowires, ANIA BLESZYNSKI, Department of Physics, Yale University — Heterostructure semi-conducting nanowires provide an excellent system to make high quality, ultra-small quantum dots for future applications in nano-electronics, spintronics, and quantum information processing. We use a liquid helium cooled scanning probe microscope (SPM) as a movable gate to image electrical conduction through an InAs quantum dot grown inside an InAs/InP heterostructure nanowire. Electrical transport measurements in the few-electron Coulomb-blockade regime exhibit the shell structure of quantum dot states down to the last electron. SPM images are formed by recording nanowire conductance as the charged SPM tip is scanned above the nanowire. The images display rings of peaked conductance centered on the quantum dot; the rings correspond to Coulomb-blockade oscillations of the quantum dot. In this way the tip locates the quantum dot and can be used as a movable gate to change the induced charge on a single dot in a spatially dependent way, down to zero electrons. We have also imaged homogeneous InAs nanowires. At 4K, the wires exhibit Coulomb blockade oscillations in conductance versus backgate voltage that are indicative of multiple quantum dots in series. The images reveal the location of the quantum dots along the wire and the tip voltage can tune their charge state.

This work was performed in collaboration with Linus Froberg, Mikael Bjork, Lars Samuelson, Floris Zwanenburg, Aarnoud Roest, Erik Bakkers, Leo Kouwenhoven, and Robert Westervelt, funded by the NSF NSEC.
11:15AM V3.00001 SQUID-detected microtesla MRI¹. MICHAEL MÖEBLE, UC Berkeley and LBNL — We have developed a system to detect nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) signals in magnetic fields of 1-100 microtesla. At such low fields, the very small nuclear polarization and the frequency dependence of conventional Faraday detection would lead to extremely weak signals. To overcome these problems we use a combination of prepolarization and frequency-independent detection with an undetuned superconducting gradiometer coupled to a Superconducting Quantum Interference Device (SQUID). We demonstrate narrow linewidths in NMR spectra of nuclei in liquids and in spectra of J-coupled nuclei in molecules. Our MRI system operates at 132 µT (proton Larmor frequency 5.6 kHz), uses a prepolarizing field up to 150 mT and has a magnetic field noise below 1 fT/Hz. Our system demonstrates millimeter in-plane resolution of phantoms, and can acquire in vivo images of the human forearm, wrist and fingers. In high-field MRI, the susceptibility difference between tissue and, for example, a medical implant, can cause severe image distortion. We show that such artifacts are absent at microtesla fields, so that this technique could enable distortion-free MRI of patients with medical implants. Furthermore, microtesla MRI displays a greatly enhanced T₁-weighted contrast between different concentrations of agarose gel (T₁ is the longitudinal relaxation time). Preliminary experiments on ex vivo prostate specimens containing normal and cancerous tissue demonstrate similarly enhanced contrast, suggesting that this technique could be used to image tumors.

¹This work was done in collaboration with S. Busch, M. Hatridge, W. Myers, S-K. Lee, R. McDermott, D. Slichter, L. Schmitt, K. Chew, J. Simko, A. Pines and John Clarke, and is supported by USDOE.

11:51AM V3.00002 Low Field Nuclear Magnetic Resonance (NMR) using SQUIDs, MARTIN BURCHOFF, Physikalisch-Technische Bundesanstalt — Using a high resolution SQUID system in a magnetically highly shielded room, we measured the precession of 1H nuclei of liquid benzene, distilled water, and chlorofom in magnetic fields around a microtesla. We found that the NMR lines of these liquids are in the range of a few hundred milliHertz and increase linearly with the detection field over a Larmor frequency range of two orders of magnitude. The slope is attributed to the inhomogeneity of the detection field and enables the extrapolation of the natural line width to zero magnetic field. For this limit, where any molecular motion is fast with respect to the Larmor frequency, the natural resonance line widths of benzene, chloroform and distilled water were determined to be 120 mHz, 150 mHz, and 170 mHz, respectively. In low magnetic fields, chemical shift and homonuclear coupling become negligible. All that remains as a source of a spectral structure is pure J-coupling between nuclei of different gyromagnetic ratio. We studied pure J-coupling between methylene protons and fluorene nuclei of trifluorethanol and between methyl protons and phosphorus in trimethylphosphate at detection fields from 0.5 microTesla to 4 microTesla. This corresponds to a variation of d=J(H,F)/(I(H)-I(F)) from 8 to 1 and of d=J(H,F)/(I(H)-I(F)) from 0.8 to 0.08, respectively. At very low fields, i.e. at d=8, the spectra of trifluorethanol exhibited only one single resonance line with an irregular structure. With increasing field, more and more individual lines were revealed. For trimethylphosphate, d=0.08 represents the transition to the weak coupling regime. In addition, we employed a 304 SQUID vector magnetometer system for the recording of the magnetic field generated by water protons in two adjacent sample tubes precessing about a magnetic field of a microTesla. From the spatially resolved data, positions and moments of the samples were calculated, yielding a reconstructed moving image of the two precessing magnetic dipoles.

12:27PM V3.00003 High resolution NMR spectroscopy in the Earth's magnetic field, STEPHAN APPELT, ZEL, FZ Juelich — High resolution nuclear magnetic resonance (NMR) spectroscopy at high magnetic fields has developed into a most powerful tool for the determination of molecular structures. The dream is a mobile molecular low field NMR scanner which allows the determination of molecular structures. Until now at low magnetic fields NMR spectroscopy suffers from the low signal to noise ratio (S/N) and from the lack of access to chemical information in terms of chemical shifts and homo-nuclear J-couplings. We demonstrate that chemical analysis of liquids is possible by mobile ultrahigh-resolution ¹H, ¹³C and ¹²⁹Xe NMR spectroscopy in the Earth’s magnetic field. The ¹²⁹Xe chemical shift in liquids is determined in the Earth’s magnetic field with a precision comparable to that obtained by superconducting magnets. The ¹H and ¹³C NMR spectra allow the determination of hetero-nuclear J-coupling constants with an accuracy of a few mHz. Very fine details of the molecular structure which are not observable with conventional superconducting magnets can be discriminated. For molecules where a rare spin such as carbon ¹³C is present the high-resolution low-field ¹H NMR spectrum indeed reveals all hetero- and homo-nuclear J-couplings. All these results open the door for the mobile study of molecular structures as well as for the online monitoring of chemical reactions at ultra-low magnetic fields.

1:03PM V3.00004 Simultaneous Measurement of Magnetic Resonance and Neuronal Signals, MICHELLE ESPY, Los Alamos National Laboratory — Nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) at ultra low magnetic fields (ULF, ~ microT) have advantages over their counterparts at higher magnetic fields, despite the reduction in signal strength. Among these advantages are that the instrumentation uses superconducting quantum interference devices (SQUIDs), and is now compatible with simultaneous measurements of biomagnetic signals, such as magnetoencephalography (MEG). This presents a new opportunity for noninvasive simultaneous functional and anatomical brain imaging. We present here the physical basis and experimental evidence for a variety of ULF-MRI techniques being developed at Los Alamos to enable simultaneous anatomical and functional imaging of the human brain. We conclude by presenting a novel technique, based on the resonant interaction between the magnetic fields such as those that arise from neural activity and the spin population in ULF-MRI experiments, that may enable direct tomographic imaging of the consequences of neural activity and functional imaging of the human brain. We conclude by presenting a novel technique, based on the resonant interaction between the magnetic fields such as those that arise from neural activity and the spin population in ULF-MRI experiments, that may enable direct tomographic imaging of the consequences of neural activity.

1:39PM V3.00005 Optical methods for detection of nuclear magnetic resonance, MICHAEL ROMALIS, Princeton University — Nuclear magnetic resonance is commonly detected with inductive pick-up coils or, less commonly, with SQUID magnetometers. I will discuss recent work in our group on optical detection of NMR using two separate techniques. In one approach, optically-pumped alkali-metal atoms are used to detect the magnetic fields generated by nuclear magnetic moments. Such atomic magnetometers reach sensitivity similar to low-T₆ SQUID magnetometers with a large dynamic range and high precision. We recently demonstrated atomic magnetometer detection of NMR and NQR signals at frequencies ranging from 20 Hz to 423 kHz. In the other approach, NMR signals from a transparent substance are obtained by direct optical detection. In this technique the plane of polarization of a source of a spectral structure is pure J-coupling between nuclei of different gyromagnetic ratio. We studied pure J-coupling between methylene protons and fluorene nuclei of trifluorethanol and between methyl protons and phosphorus in trimethylphosphate at detection fields from 0.5 microTesla to 4 microTesla. This corresponds to a variation of d=J(H,F)/(I(H)-I(F)) from 8 to 1 and of d=J(H,F)/(I(H)-I(F)) from 0.8 to 0.08, respectively. At very low fields, i.e. at d=8, the spectra of trifluorethanol exhibited only one single resonance line with an irregular structure. With increasing field, more and more individual lines were revealed. For trimethylphosphate, d=0.08 represents the transition to the weak coupling regime. In addition, we employed a 304 SQUID vector magnetometer system for the recording of the magnetic field generated by water protons in two adjacent sample tubes precessing about a magnetic field of a microTesla. From the spatially resolved data, positions and moments of the samples were calculated, yielding a reconstructed moving image of the two precessing magnetic dipoles.

Thursday, March 8, 2007 11:15AM - 2:15PM — Session V5 DCMP: Unusual Transport Phenomena in Chalcogenides Colorado Convention Center Korbel 1A-1B

11:15AM V5.00001 Quantum Linear Magnetoresistance: Solution of an Old Mystery, A.A. ABRIKOSOV, Argonne National Laboratory — In the paper the history of the discovery of the linear magnetoresistance in metals by P. L. Kapitza in 1928 - 1929 and its explanations are presented. Actually, Kapitza discovered two different phenomena. One of them — the linear magnetoresistance at classically large magnetic fields in polycrystalline samples of metals, having open Fermi surfaces, was explained by I. Lifshits and V. Peschansky in 1958. The other phenomenon is the quantum linear magnetoresistance, appearing in metals, or semimetals, with a small concentration of carriers and a small effective mass, when only the lowest Landau band participates in the conductivity. Manifestations of this unusual phenomenon in different materials are described.
11:51AM V5.00002 The quest for imperfection. ANIKE HUSMANN, Cambridge University — The stoichiometric compounds \( \text{Ag}_2\text{S}, \text{Ag}_2\text{Se} \) and \( \text{Ag}_2\text{Te} \) are superionic conductors at higher temperature. Below 400 K, ion migration is effectively frozen and the compounds are non-magnetic semiconductors that exhibit no appreciable magnetoresistance. We showed that slightly altering the stoichiometry can lead to a marked increase in the magnetic response; up to 200% at room temperature and in a magnetic field of 5.5T in \( \text{Ag}_2\text{Se} \) and \( \text{Ag}_2\text{Te} \) (4 about 10^{-4} reaching a maximum of about 350% at low temperature. But more importantly, the response can be almost linear in magnetic field even at low magnetic fields. Not only do these silver chalcogenides show linear magnetoresistance, this response also is still saturating up to 55T showing no signs of saturation. M. Parish and P. Littlewood identified this effect as a key feature. Their theoretical model has initiated a project on artificially created structures in semiconductors to mimic transport in real materials with inhomogeneities. We processed a number of different geometric realizations in collaboration with L. Cohen’s group at Imperial College, London, on their InSb epilayers on GaAs (001). However, the films themselves have a very large and almost linear and non-saturating (up to applied fields of 13 T) magnetoresistance intrinsically which made the interpretation of the results somewhat difficult. We then went back to the origin of this intrinsic magnetoresistance by comparing, at room temperature, undoped InSb epilayers grown on GaAs(001) by molecular-beam epitaxy with varying thickness from 100 to 2000nm. The question is whether these films and the silver chalcogenides share a similar physical origin for their magnetoresistance. Experiments to very high fields in InSb films are on the way.

12:27PM V5.00003 Non-saturating magnetoresistance in heavily disordered semiconductors. MEERA PARISH, Princeton University — We present a classical model of the magnetotransport of strongly inhomogeneous semiconductors based on an array of coupled four-terminal elements. We show that this model generically yields non-saturating, quasi-linear magnetoresistance at large magnetic fields, in contrast to the resistance of a homogeneous semiconductor, which increases quadratically with magnetic field at low fields and, except in very special cases, saturates at fields much larger than the inverse of the carrier mobility. We argue that our model provides an explanation for the observed non-saturating magnetoresistance in doped silver chalcogenides and potentially in other macroscopically disordered conductors. Finally, our method may be used to design the magnetoresistance response of a microfabricated array and thus pave the way to the construction of magnetic field sensors with a controllable response.

1:03PM V5.00004 The Evolution from CDW to Superconductivity in \( \text{Cu}_x\text{TiSe}_2 \). ROBERT CAVA, Department of Chemistry, Princeton University — Charge density waves (CDWs) are periodic modulations of the conduction electron density in solids: collective states that arise due to intrinsic instabilities often present in low dimensional electronic systems. The layered dichalcogenides are the most well known examples of CDW-bearing systems, and \( \text{TiSe}_2 \) was one of the first CDW-bearing materials known. The competition between CDW superconducting states at low temperatures has often been characterized and discussed, and yet no chemical system has been previously reported where finely controlled chemical tuning allows for this competition to be studied in detail. This talk will describe our work [1] reporting how, upon controlled intercalation of \( \text{TiSe}_2 \) with \( \text{Cu} \) to yield \( \text{Cu}_x\text{TiSe}_2 \), the CDW transition is continuously suppressed, and a new superconducting state emerges near \( x = 0.04 \), with a maximum \( T_c \) of 4.15K found at \( x = 0.08 \). The anisotropic superconducting properties, obtained by characterization of the resistivity and magnetization of single crystals of \( \text{Cu}_{0.07}\text{TiSe}_2 \), will also be described.


Work supported by the Dept. of Energy, Solid State Chemistry program.

1:39PM V5.00005 Current Jets and Non-saturating Magnetoresistance in Disordered Semiconductors. JINGSHI HU, University of Chicago — The transverse, positive magnetoresistance of doped silver telluride and silver selenide changes linearly with field by thousands of percent, with no sign of saturation up to MegaGauss. The inhomogeneous distribution of excess/deficient silver atoms lies behind this anomalous magnetoresistive response, introducing spatial conductivity fluctuations with length scales independent of the cyclotron radius. Theoretical simulations of two and three-dimensional random resistor networks reveal distorted current flows that provide a linear contribution to the transverse magnetoresistance, but a pronounced negative longitudinal magnetoresistance. We show that a systematic investigation of the resistivity tensor in longitudinal fields could be used to identify the spatial inhomogeneities in the silver chalcogenides and determine the associated length scale of the current distortion. The incorporation of macroscopic inhomogeneities to other semiconductors, such as InSb, opens the gate to artificial fabrication of conducting networks with micron scale unit size for enhanced magnetoresistive sensitivity.


Thursday, March 8, 2007 11:15AM - 1:51PM
Session V8 DCMP: Superconductivity: Spin Excitations and Ordering in Cuprates
Colorado Convention Center Korbel 1C

11:15AM V8.00001 Antiferromagnetism and superconductivity do not seem to coexist in \( \text{Nd}_{2−x}\text{Ce}_x\text{CuO}_4 \pm \delta \). EUGENIE MOOTOYAMA, GUICHUAN YU, INNA VISHIK, Stanford University, OWEN VAJK, University of Missouri, PATRICK MANG, MARTIN GREVEN, Stanford University — High transition-temperature (\( T_c \)) superconductivity develops near antiferromagnetic (AF) phases, and it is possible that magnetic excitations contribute to the superconducting (SC) pairing mechanism. In order to assess the role of antiferromagnetism, it is essential to understand the doping dependence of the two-dimensional AF spin correlations. The phase diagram is asymmetric with respect to electron and hole doping, and for the comparatively less-studied electron-doped materials, the AF phase extends much further with doping and it appears to overlap with the SC phase: the archetypical compound \( \text{Nd}_{2−x}\text{Ce}_x\text{CuO}_4 \pm \delta \) shows bulk superconductivity above \( x = 0.13 \), while evidence for AF order has been found up to \( x = 0.17 \). However, our inelastic magnetic neutron scattering measurements point to the distinct possibility that genuine long-range antiferromagnetism and superconductivity do not co-exist. The data reveal a magnetic quantum critical point where superconductivity first appears, consistent with an exotic quantum phase transition between the two phases. Our measurements also demonstrate that the pseudogap phenomenon in the electron-doped materials arises from a build-up of spin correlations, in agreement with recent theoretical proposals.

11:27AM V8.00002 New phase diagram of ideally flat \( \text{Cu}_2 \) plane. Cu-NMR study in Five-layered Cuprates. HIDEKAZU MUKUDA, Osaka University, MACHIKO ABE, SUNAO SHIMIZU, YOSHIO KITAOKA, AKIRA IYO, HIJIRI KITO, YASUMOTO TANAKA, YASUHARU KODAMA, KAZUYASU TOKIWA, TSUNEICHI SAWABE, OKAZAKI UNIVERSITY TEAM, NATIONAL INSTITUTE OF ADVANCED INDUSTRIAL SCIENCE AND TECHNOLOGY (AIST) TEAM, TOKYO UNIVERSITY OF SCIENCE TEAM — We report a systematic Cu-NMR study on \( \text{Hg}_2\text{Bi}_2\text{Ca}_2\text{Cu}_3\text{O}_{x+} \) with a Tc=72K, while evidence for AF order has been found up to \( x = 0.17 \). However, our inelastic magnetic neutron scattering measurements point to the distinct possibility that genuine long-range antiferromagnetism and superconductivity do not co-exist. The data reveal a magnetic quantum critical point where superconductivity first appears, consistent with an exotic quantum phase transition between the two phases. Our measurements also demonstrate that the pseudogap phenomenon in the electron-doped materials arises from a build-up of spin correlations, in agreement with recent theoretical proposals.

11:39AM V8.00003 High-Tc superconductivity and antiferromagnetism on self-doped high-Tc cuprate Ba2Ca2Cu3O8+x. SUNAO SHIMIZU, HIDEKAZU MUKUDA, YOSHIKOSHI KITAOKA, Osaka University, AKIRA IYO, YASUHARU KODAMA, HUJIRI KITO, National Institute of Advanced Industrial Science and Technology, KAZUYASU TOWKIA, TSUNEI WATANABE, Tokyo University of Science — We report on the antiferromagnetism and high-Tc superconductivity in a F-substituted four-layered cuprate, composed of two outer and inner CuO2 planes in a unit cell, Ba2Ca2Cu3O8+x. Although a formal Cu valence is expected to be just +2.0 in the nominal composition, this is not a half-filled Mott insulator but a superconductor with Tc = 55K. Recently, it has been suggested that the origin of the superconductivity in this compound is self-doping by ARPES measurement [1] and band calculation [2], which means either outer or inner CuO2 planes are hole-doped, and the others are electron-doped. From F-NMR study, we have confirmed magnetic order with T' = 100K, concluding the uniform mixing of superconductivity and magnetic order in a single CuO2 plane. In addition, we have compared a three-layered compound Ba2Ca2Cu3O8+x, which is also superconductor with Tc = 76K. We will introduce the unique magnetic and superconducting phenomena in F-substituted cuprates from microscopic points of view. [1] Y. Chen, et al., cond-mat/0611291 (2006) [2] W. Xie, et al., cond-mat/0607198 (2006)

11:51AM V8.00004 Effect of oxygen ordering on the spin dynamics of YBa2Cu3O6.5. SHILIANG LI, University of Tennessee, Z. YAMANI, Chalk River Laboratories, Canada, H.J. KANG, NIST Center for Neutron Research, FENG YE, Oak Ridge National Laboratory, C. BIRCHER, University of Tennessee, K. SEGAWA, Y. ANDO, Central Research Institute of Electric Power Industry, Japan, XIN YAO, Shanghai Jiao Tong University, China, H.A. MOOK, Oak Ridge National Laboratory, PENGCHENG DAI, University of Tennessee — We use inelastic neutron scattering to study the oxygen disorder effect in electronic properties of YBCO 6.5. Previous work have shown when copper oxygen chains in the YBCO 6.5 form ortho-II order, magnetic excitations in YBCO6.5 form a resonance around 33 meV and incommensurate spin fluctuations below the resonance. In order to study oxygen disorder effect on spin excitations of YBCO 6.5, we measured spin dynamics of detwinned Ortho-I YBCO(x=6.5) (Tc=48K), whose Cu-O chains are not well ordered. We find that oxygen disorder can have dramatic effect on spin dynamics of YBCO6.5. We discuss similarities and differences in spin dynamics in these two materials and their possible interpretation.

12:03PM V8.00005 Evolution of hourglass like magnetic excitation in underdoped La1-xSr1+xCuO4. MAIKO KOFU, Univ. of Virginia, TETSUYA YOKOO, KEK, KAZUYOSHI YAMADA, Tohoku Univ., FRANS TROUW, LANL — Recent neutron scattering studies have revealed similar "hourglass-like" magnetic excitations in mono-layered La1.875Ba0.125CuO4 and bi-layered YBa2Cu3O6.5. These results indicate that such hourglass-like dispersive excitations might be common to high-Tc cuprates. To elucidate the interplay between the excitation and the superconductivity, we investigated the hole doping dependence of excitations. We performed inelastic neutron experiments for underdoped La1.90Sr0.10CuO4 (Tc=29K) using chopper spectrometer PHAROS installed at Los Alamos National Laboratory. Clear four incommensurate peaks were observed at ω=8meV and the incommensurability corresponds to ~0.1 r.l.u., which is consistent with previous study. Around ω=30meV, a single peak was observed at the antiferromagnetic magnetic zone center. This indicates that the hourglass-like excitations also exist in underdoped La1.90Sr0.10CuO4 and that the saddle point becomes ~30meV. For optimally doped La1.84Sr0.16CuO4(Tc=38K), the saddle point is expected to correspond to 40meV or more, suggesting that the saddle point goes up with increasing hole doping. Moreover, we found that the slope of dispersion is almost same for La1.90Sr0.10CuO4 and La1.84Sr0.16CuO4. The reduction of energy at saddle point is recognized as a consequence of difference of incommensurability.

12:15PM V8.00006 Neutron Scattering in High-Tc Cuprates: Two Component Spin-Fermion Model. YUNKYU BANG, Chonnam National University — Recent neutron scattering experiments reveal that the generic form of the magnetic excitations in the high-Tc cuprates has the so-called "hourglass" form, in which both the quasi-static incommensurate (IC) excitations and the incommensurate resonance peak show up at different excitation energies. We propose the two-component spin-fermion model having the local spin degrees of freedom and itinerant fermions. Our calculations of the dynamic spin correlation function both at normal and superconducting states explain the essential features of the hour-glass form of the neutron experiments.

12:27PM V8.00007 Inelastic neutron scattering study on spin excitations of Pr0.85LaC8O9.12Cu1.8 (Tc=27.5K). JUN ZHAO, SHILIANG LI, STEPHEN WILSON, University of Tennessee, HYE JUNG KANG, JEFF LYNN, NIST Center for Neutron Research, PENGCHENG DAI, University of Tennessee — We use neutron scattering to study the evolution of spin excitations in electron doped Pr0.85LaC8O9.12Cu1.8 (PLCCO). For Tc = 24 K PLCCO, Wilson et al. [Nature 442, 59 (2006)] have reported the presence of a resonance mode, a localized magnetic excitations coupled directly to the superconductivity in high-Tc superconductors, similar to hole-doped superconductors such as YBa2Cu3O6.5, Bi2Sr2CaCu2O8 +δ and Tl2Ba2CaCu2O8 +δ. Below the resonance are continuing magnetic scattering with little temperature dependence. We show here our studies of the magnetic excitations on PLCCO (Tc=27.5K) with the highest Tc reported in the literature. We confirm the presence of a resonance mode in this sample, and demonstrate that the low-energy magnetic scattering here is much different from the Tc=24 K PLCCO. Our results thus shed new light to the understanding of spin excitations in electron-doped copper oxides.

12:39PM V8.00008 Spin wave excitations in Nd2CuO4. CHAD BIRCHER, HYUNJGE WOO, SHILIANG LI, PENGCHENG DAI, University of Tennessee — In this talk we will present the Nd neutron scattering results of spin wave excitations of the electron-doped superconductor parent compound Nd2CuO4 (NCO). We carried out our experiments on the HET time of flight spectrometer at the ISIS facility in England. Our work will complement previous studies on the parent compound of hole-doped superconductors, La2CuO4 (LCO). We are studying whether there is a difference between the magnetic exchange coupling of hole-doped and electron-doped superconductors. We have probed energies from 50 meV to above 300 meV in order to determine the magnetic exchange coupling. We will present the results and discuss the similarities and differences between LCO and NCO.

12:51PM V8.00009 Incommensurate Spin Ordering and Excitations in Underdoped La2−xSrxCuO4. S.R. DUNSIGER, Y. ZHAO, B.D. GAULIN, Dept of Physics and Astronomy, McMaster University, Hamilton, Canada, Y. QIU, J.R.D. COPLEY, NIST Center for Neutron Research, Gaithersburg, USA, H.A. DABKOWSKA, Dept of Physics and Astronomy, McMaster University, Hamilton, Canada, Z. YAMANI, W.J.L. BUYERS, Canadian Neutron Beam Centre, NRC, Chalk River, Canada — The diverse magnetic properties of the La2−x(Sr,Ba)CuO4 transition metal oxides may be tuned in a controllable way by doping with mobile holes. In one interpretation, the holes are believed to organise into correlated static or dynamic stripes. We report the first observation of static incommensurate spin ordering in underdoped La2−xBa1−xCuO4 (x<0.05, x=0.08) using neutron diffraction. Elastic collinear incommensurate peaks are observed below the superconducting transition (Tc ~27 K) in La2−x(Sr,Ba)CuO4 (x=0.08). In marked contrast, diagonal satellite peaks have been observed at low temperature in positions rotated by 45° within the (HKO) plane for La2−x(Sr,Ba)CuO4 (x~0.05). Our neutron scattering results are compared with analogous studies on La2−xSrCuO4 which indicate that such a rotation of the spin structure may be a generic feature of the underdoped La2−214 cuprates.
Spin and Charge Excitations in Checkerboards based on a Superstructure

DAVID K. CAMPBELL, DAOXIN YAO, Departments of Physics and Electrical and Computer Engineering, Boston University, ERICA W. CARLSON, Department of Physics, Purdue University — Checkerboard patterns have been proposed to explain the real space structure observed in STM experiments on BSCO and Na-CCCO. However, simple checkerboard patterns always give incommensurate (IC) spin peaks rotated 45 degrees from the direction of the charge IC peaks, contrary to what is seen in neutron scattering. [1] Here, we study a more complicated checkerboard pattern which can resolve the low frequency inconsistency. Using spin wave theory, we explore the finite frequency response of this superstructure and find that the high energy response is inconsistent with neutron scattering results. In particular, there is no spin resonance peak.


Connecting spin and charge response in electron-doped cuprates

ANDREAS SCHNYDER, Condensed Matter Theory Group, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland, DIRK MANSKÉ, Max Planck Institut fuer Festkorperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — We perform a detailed analysis of angle-resolved photoemission data from electron-doped cuprates [1,2] in order to extract both the self-energy and the bare dispersion of the quasiparticles. The self-energy contains important information about the interactions among the quasiparticles. Taking the extracted bare quasiparticle dispersion as an input parameter we compute dynamical response functions employing a spin-fluctuation-based theory. In particular we estimate the dynamical spin susceptibility, which we then compare to recent inelastic neutron scattering data [3]. We obtain a resonance at the anti-ferromagnetic ordering wavevector (π, π), whereas incommensurate spin excitations are mostly suppressed. Our approach provides a consistent theoretical description of both the spin and charge response in electron-doped cuprates.


Local moment and inhomogeneous hyperfine interaction in the CuO2 plane of Bi2Sr2CaCuO6+δ (Bi2212) single crystal by 17O NMR

BO CHEN, SUTIRTHA MUKHOPADHYAY, WILLIAM HALPERIN, Northwestern University, PRASENJIT GUPTASARMA COLLABORATION, DAVID G. HINKS COLLABORATION — The 17O NMR spectra of Bi2Sr2CaCuO6+δ (Bi2212) single crystals were measured in the magnetic field of 8 T from 4 K to 200 K. The linewidth of the oxygen in CuO2 plane, O(1), was found to follow a Curie temperature dependence in the normal state, where the Curie coefficient decreases with the increase of δ oxygen in the crystal. In the superconductive state, it decreases with decreasing temperature, proportional to the decreasing Knight shift. This temperature dependence of the linewidth identifies the existence of local moment and inhomogeneous hyperfine interaction in the CuO2 plane.

1University of Wisconsin-Milwaukee
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Low-energy spin dynamics in La2+0.05Sr1-xCuO4

WEI BAO, Los Alamos National Lab., YING GASPAROVIC, NIST, KASU YAMADA, Tohoku Univ., Japan, EMILIO LORENZO, CNRS, Grenoble, France, J-H. CHUNG, NIST — The hypothesis that the vortex lattice induced by perpendicular magnetic field in films of PLD-(La,Ba)2CuO4 is in a thermodynamic Bose glass state accounts for the inverse-square-root power law shown by the critical current density versus perpendicular magnetic field. In particular, a broken glass state is characterized by the existence of local moment and inhomogeneous hyperfine interaction in the CuO2 plane.

1:03PM V8.00010 Spin and Charge Excitations in Checkerboards based on a Superstructure

1:15PM V8.00011 Connecting spin and charge response in electron-doped cuprates

1:27PM V8.00012 Local moment and inhomogeneous hyperfine interaction in the CuO2 plane of Bi2Sr2CaCuO6+δ (Bi2212) single crystal by 17O NMR

1:39PM V8.00013 Low-energy spin dynamics in La2+0.05Sr1-xCuO4

The interesting differences between the low-temperature vortex liquid in La2−xSrxCuO4 and Bi2Sr2−yLa1yCuO6

LU LI, YAYU WANG, JOSEPH G. CHECKELSKY, Physics Department, Princeton University, SEIKI KOMIYA, SHIMPEI ONO, YOICHI ANDO, Central Research Institute of Electric Power Industry, Japan, NAI PHUAN OONG, Physics Department, Princeton University — Diamagnetism in lightly-doped crystals of La2−xSrxCuO4 (LSCO) with doping x = 0.03 to 0.09 has been investigated by torque magnetometry, which resolves weak 2D supercurrents against a nearly isotropic paramagnetic spin response. By carefully subtracting the large paramagnetic susceptibilities of the van Vleck and spin terms, we observe the diamagnetic signal of vortices in fields up to 45 T, even for x as low as 0.03. The torque results allow the x dependence of both the melting field Hc2 and upper critical field Hc2 to be measured. We find that Hc2 extends smoothly across the critical doping value xc ≃ 0.055. Below xc, the pair condensate survives as a vortex liquid in intense fields, but long-range phase coherence is absent down to our lowest temperature T = 0.35 K. We discuss the interesting differences between the vortex liquid and solid phases, and the collapse at low T of phase coherence at the boundary. The close correlation of T onset to Hc2 in LSCO and Bi2201 will also be reported. Research supported by NSF grant DMR 0213706.

1Supported by the Air Force Office of Scientific Research, grant no. FA9550-06-1-0479.

1:03PM V8.00010 Spin and Charge Excitations in Checkerboards based on a Superstructure

1:15PM V8.00011 Connecting spin and charge response in electron-doped cuprates

1:27PM V8.00012 Local moment and inhomogeneous hyperfine interaction in the CuO2 plane of Bi2Sr2CaCuO6+δ (Bi2212) single crystal by 17O NMR

1:39PM V8.00013 Low-energy spin dynamics in La2+0.05Sr1-xCuO4

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1Supported by the Air Force Office of Scientific Research, grant no. FA9550-06-1-0479.

11:15AM V9.00001 Does a Bose-Glass State Exist in Commercial High-Tc Wires?1

JOSE P. RODRIGUEZ, California State University at Los Angeles — The hypothesis that the vortex lattice induced by perpendicular magnetic field in films of PLD-YBCO is in a thermodynamic Bose glass state accounts for the inverse-square-root power law shown by the critical current density versus perpendicular magnetic field. We study here how robust such a state is to the addition of point pinning centers. This is done by first calculating the tilt modulus of the “pristine” Bose-glass state. It is found to diverge at long-wavelength along the magnetic-field/correlated-defect direction. A Larkin-Ovchinnikov analysis then yields a 2D/3D phase transition in collective pinning that is first-order. In particular, a broken Bose glass state characterized by finite Larkin domains, within which correlated pinning centers remain effective, exists at strong enough point pinning, at small enough coherence lengths. A signature of the broken glass state is the existence of local moment and inhomogeneous hyperfine interaction in the CuO2 plane.

1Supported by the Air Force Office of Scientific Research, grant no. FA9550-06-1-0479.

11:27AM V9.00002 The low-temperature vortex liquid in La2−xSrxCuO4 and Bi2Sr2−yLa1yCuO6

LU LI, YAYU WANG, JOSEPH G. CHECKELSKY, Physics Department, Princeton University, SEIKI KOMIYA, SHIMPEI ONO, YOICHI ANDO, Central Research Institute of Electric Power Industry, Japan, NAI PHUAN OONG, Physics Department, Princeton University — Diamagnetism in lightly-doped crystals of La2−xSrxCuO4 (LSCO) with doping x = 0.03 to 0.09 has been investigated by torque magnetometry, which resolves weak 2D supercurrents against a nearly isotropic paramagnetic spin response. By carefully subtracting the large paramagnetic susceptibilities of the van Vleck and spin terms, we observe the diamagnetic signal of vortices in fields up to 45 T, even for x as low as 0.03. The torque results allow the x dependence of both the melting field Hc2 and upper critical field Hc2 to be measured. We find that Hc2 extends smoothly across the critical doping value xc ≃ 0.055. Below xc, the pair condensate survives as a vortex liquid in intense fields, but long-range phase coherence is absent down to our lowest temperature T = 0.35 K. We discuss the interesting differences between the vortex liquid and solid phases, and the collapse at low T of phase coherence at the boundary. The close correlation of T onset to Hc2 in LSCO and Bi2201 will also be reported. Research supported by NSF grant DMR 0213706.

1Present address:University of California,Berkeley
11:39AM V9.00003 High-frequency response of Josephson vortex lattice in layered superconductors\(^1\), ALEXEI KOSHELEV, Argonne National Laboratory — Magnetic field applied along the layer direction of layered superconductors generates the Josephson vortex lattice. We studied response of this state to the high-frequency c-axis electric field. Numerically solving equations for the oscillating phases, we computed the frequency dependences of the loss function, Im\[1/\omega\mid\], at different magnetic fields, including regions of both dilute and dense Josephson vortex lattices. The main feature of the response is the Josephson-plasma-resonance peak. In the dilute-lattice regime this peak is displaced to slightly lower frequency. An interesting feature of the dilute regime is the appearance of satellites at the higher-frequency part, which are caused by excitation of the plasma modes with the wave vectors set by the lattice structure. In the dense-lattice limit the plasma peak moves to higher frequency and its intensity rapidly decreases, in agreement with analytical theory. An additional broad peak exists at low frequencies, and can be described by phenomenological theory of vortex oscillations.

\(^1\)This work was supported by the U. S. DOE, Office of Science, under contract # DE-AC02-06CH11357

11:51AM V9.00004 Universality in the Self Organized Critical behavior of a cellular model of superconducting vortex dynamics\(^1\), YUDONG SUN\(^2\), TEGY VADAKKAN, KEVIN BASSLER, The University of Houston — We study the universality and robustness of variants of the simple model of superconducting vortex dynamics first introduced by Bassler and Paczuski in Phys. Rev. Lett. 81, 3761 (1998). The model is a coarse-grained model that captures the essential features of the plastic vortex motion. It accounts for the repulsive interaction between vortices, the pinning of vortices at quenched disordered locations in the material, and the over-damped dynamics of the vortices that leads to tearing of the flux line lattice. We report on the results of extensive simulations of the critical “Bean state” dynamics of the model. We find a phase diagram containing four distinct phases of dynamical behavior, including two phases with distinct Self Organized Critical (SOC) behavior. Exponents describing the avalanche scaling behavior in the two SOC phases are determined using finite-size scaling. The exponents are found to be robust within each phase and for different variants of the model. The difference of the scaling behavior in the two phases is also observed in the morphology of the avalanches.

\(^1\)The authors acknowledge support from the NSF through grant No. DMR-0427538

\(^2\)Membership Pending

12:03PM V9.00005 Molecular Dynamics simulations of the vortex matter two-stage melting transition in Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_y\) in the presence of straight and of tilted columnar defects\(^1\), JIN-TAO LIU, YADIN Y. GOLDSCHMIDT, University of Pittsburgh — In this paper we use London Langevin molecular dynamics simulations to investigate the vortex matter melting transition in the highly anisotropic high-temperature superconductor material Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_y\) in the presence of low concentration of columnar defects (CDs). We reproduce with further details our previous results obtained by using Multilevel Monte Carlo simulations that showed that the melting of the nanocrystalline vortex matter occurs in two stages: a first stage melting into nanoliquid vortex matter and a second stage delocalization transition into a homogeneous liquid. Furthermore, we report on new dynamical measurements in the presence of a current that identifies clearly the second stage delocalization transition. In addition to CDs aligned along the c-axis we also simulate the case of tilted CDs which are aligned at an angle with respect to the applied magnetic field. Results for a 45\(^\circ\) tilt of the CDs show that the location of the melting transition is not affected by the tilt when the ratio of flux lines to CDs remains constant.

\(^1\)Supported by the US department of Energy (DOE), the NERSC program and the Pittsburgh Supercomputing Center.

12:15PM V9.00006 Disparities in the vortex state electrodynamics of high Tc cuprates, ANDREW LAFORGE, ZHIQIANG LI, University of California, San Diego, WILLIE PADILLA, KENNETH BURCH, Los Alamos National Laboratory, SASA DORDEVIC, University of Akron, KOUI SEGAWA, YOICHI ANDO, Central Research Institute of Electric Power Industry, Japan, DIMITRI BASOV, University of California, San Diego — We report new far infrared measurements of underdoped YBCO in magnetic field and situate these new data within earlier work on related compounds. We show that the cuprate superconductors, including YBa\(_2\)Cu\(_3\)O\(_y\) (YBCO), La\(_2-x\)Sr\(_x\)CuO\(_4\) (LSCO), and Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_y\) (BSCCO), have revealed strikingly different vortex state electric dynamic responses between the various families. For example, in the Josephson vortex regime a strongly field dependent transverse resonance is observed in the interplane conductivity of YBCO, whereas no such feature is found in LSCO. Microwave magnetoabsorption spectra of BSCCO exhibit two resonances which are separated by a temperature gap, again at variance with the other systems. We compare and contrast these findings with several models of the electrodynamics in the vortex state and offer possible explanations for the observed discrepancies.

12:27PM V9.00007 Magnetic measurement of RF-induced flux lattice annealing (RFILA) in the electron-doped superconductor Pr\(_{1.85}\)Ce\(_{0.15}\)CuO\(_4-y\), W.G. CLARK, G. GAIDOS, G. WU, S.E. BROWN, UCLA Physics and Astronomy, R.L. GREENE, U. of Maryland Physics, H. BALCI, UIUC Physics — A strained flux lattice (FL) in a superconductor (SC) can be annealed to a lower free energy by the RF-field used to generate an NMR spin-echo signal [W.G. Clark et al., J. Phys. IV Proceedings 9, P10.49-52 (1999)]. Here, we report the change in the rf magnetic susceptibility (\(\chi\)) in the SC phase of a single crystal of Pr\(_{1.85}\)Ce\(_{0.15}\)CuO\(_4-y\) with a strained FL by successive RFILA pulses. The distorted FL is prepared by rotating the sample through a small angle in a magnetic field well below the SC transition temperature, leaving the FL pinned in a non-equilibrium configuration. RFILA pulses then reduce \(\chi\), which is measured by the change in the inductance of a coil surrounding the sample using an NMR probe and spectrometer. The interpretation is that shaking the FL by the RF pulses progressively annihilates it to a lower free energy configuration, which has a smaller \(\chi\). These measurements provide a very sensitive measure of the RFILA effect. Work at UCLA was supported by NSF Grants DMR-0334869 (WGC) and DMR-0520552 (SEB).

12:39PM V9.00008 ABSTRACT WITHDRAWN —

12:51PM V9.00009 Puzzling magnetic behavior of non-centrosymmetric superconductor Re\(_3\)W, V. KUZNETSOVA, University of Tennessee, J.R. THOMPSON, University of Tennessee, ORNL, Y. ZUEV, D.K. CHRISTEN, R. JIN, ORNL — We have studied magnetic properties of non-centrosymmetric superconductor Re\(_3\)W. Unlike ordinary BCS superconductors, annealed samples of Re\(_3\)W exhibit linear Abrikosov-like dependence of the equilibrium (\(M_{eq}\)) and non-equilibrium (\(M\)) magnetization on magnetic field \(H\) in an anomalously large range \(H \approx (0.1-1)H_{c2}\). This behavior is drastically different for the quenched (“as prepared”) samples of Re\(_3\)W. Equilibrium magnetization was obtained by “shaking” the flux line lattice with an alternating transverse field. \(M_{eq}\) curves show change in slope in about the same region of magnetic fields where the slopes of corresponding critical currents \(J_c(H)\) also change. In our talk, we discuss probable causes of these effects. ORNL is managed by UT-Battelle, LLC for USDOE under contract DE-AC05-00OR22725.
1:03PM V9.00010 Ground state of interlayer Josephson vortex systems and the shear modulus, YOSHIHIKO NONOMURA, XIAO HU, Computational Materials Science Center, National Institute for Materials Science, Tsukuba, Ibaraki 305-0047, Japan — Ground state of interlayer Josephson vortex systems is investigated on the basis of the full Lawrence-Doniach model. We find: (1) For low fields, field dependence of $c_{66}$ approximately coincides with the elastic theory, and jumps in $c_{66}$ correspond to the structural phase transitions between various rotated-lattice configurations. (2) For intermediate fields, the ground state is characterized by continuously-varying shear angle of vortex lattices. In this region $c_{66}$ becomes smaller than those in the elastic theory, and vanishes at the shear instability field. This critical field is increased by inhomogeneity of the magnetic field. (3) For high fields, $c_{66}$ converges to a constant value, which is quite different from the exponentially-decaying $c_{66}$ in the London theory. This saturation of $c_{66}$ can be interpreted as the effect of “effective core size” within the elastic theory, and is not affected by inhomogeneity of the superconducting amplitude for material parameters of cuprate high-$T_c$ superconductors.

1:15PM V9.00011 Thermal study of vortex states in mesoscopic superconducting disks$^1$. FLORIAN ONG, OLIVIER BOURGEOIS, CNRS-Institut Neel, SERGEY SKIPETROV, CNRS-LP2MC, JACQUES CHAUSSY, CNRS-Institut Neel — We present low temperature highly sensitive heat capacity $C$ measurements$^{[1,2]}$ of aluminum disks with diameters close to $\xi(T)$, the superconducting coherence length. $C(T)$ scans under fixed perpendicular magnetic fields $H$ reveal a quasiperiodic modulation of the height $\Delta C$ of the $C$ jump at the superconducting to normal phase transition. This behavior is due to transitions between several arrangements of vortices in the disks. Indeed giant vortex states or multivortex states can be observed, with a vorticity (an integer equal to the number of vortices threading a single disk) depending on $H$, $T$, and on the size of the disks. Heat capacity measurements enable to study phase transitions between such states, without contacting or biasing them. Thus phase boundaries in the $H-T$ plane can be drawn in all the superconducting region.

$^1$This work was supported by the Région Rhône-Alpes and the IPMC Grenoble

1:27PM V9.00012 Vortex Lattice Structural Transitions: A generalized (thermal fluctuations and quench disorder) Ginzburg-Landau Approach, PEI-JEN LIN, National Chiao Tung University, GOLAN BEL, BARUCH ROSENSTEIN — Base on Guzburg-Landau model, we study the rhombic-to-square transition for tetragonal material in the magnetic fields along $c$ axis with the account of thermal fluctuation and disorder influence. The new perturbative approach is used to approach the melting line of vortex lattice. The result will compare with the recent neutron scattering data and second peak effect on high $Tc$. SC and Low $Tc$. SC.

1:39PM V9.00013 ABSTRACT HAS BEEN MOVED TO J8.00012

1:51PM V9.00014 Deconfinement of Vortices with Continuously Variable Fractions of the Unit Flux Quanta in Two-Gap Superconductors$^1$, JUN GORYO, Aoyama Gakuin University, SINGO SOMA, HIROSHI MATSUAWA, Aoyama Gakuin University — We propose a new stage of confinement-deconfinement transition, which can be observed in laboratory. In two-gap superconductors, two kinds of vortex exist by the presence of two different $U(1)$ phases. Each of them carries a continuously variable fraction of the unit flux quanta $\Phi_0 = hc/2e$. The confined state of these two is a usual vortex and stable in the low temperature region of the system under a certain magnetic field above $H_{c1}$. We see an analogy to quarks in a charged pion. An entropy gain causes two fractional vortices to be deconfined above a certain temperature. We estimate the condition of the deconfinement by using parameters for a typical two-gap superconductor MgB$_2$.

$^1$This work is financially supported by Grant-in-Aid for Scientific Research from Japan Society for the Promotion of Science under Grant Nos.15540370, 16740226, and 18540381.

Thursday, March 8, 2007 11:15AM - 2:03PM

Session V10 DCMP: Critical and Non-equilibrium Phenomena Colorado Convention Center Korbel 1E

11:15AM V10.00001 Scaling Functions and Conformal Invariance at the Quantum Critical Point of the Sub-Ohmic Bose-Fermi Kondo Model, STEFAN KIRCHNER, QIMIAO SI, Department of Physics & Astronomy, Rice University, Houston, TX 77251 — In one approach to the quantum critical heavy fermion metals, Kondo lattice systems are studied through a self-consistent Bose-Fermi Kondo Model (BFKM) within the extended dynamical mean field theory. It has become clear in recent years that the critical behavior of the BFKMs is not captured by the classical critical theory obtained through the standard “quantum-to-classical mapping” of the model. In this work, we study the finite temperature scaling functions of the easy-axis BFKM using a cluster-updating Monte Carlo approach, and their counterparts of a spin-isotropic BFKM in a dynamical large-$N$ limit. The scaling functions are found to have the form dictated by a boundary conformal field theory even though the underlying Hamiltonian lacks conformal invariance. In the large-$N$ limit, this is established for all multiple-spin correlation functions as well. The results raise the possibility that the quantum critical point of the BFKM has an enhanced symmetry, which should be helpful to the understanding of the underlying critical field theory.

11:27AM V10.00002 Zero Bias Anomaly Out of Thermal Equilibrium, DMITRI GUTMAN, University of Florida, YUVAL GEFEN, Weizmann Institute of Science, ALEXANDER MIRLIN, University and Forschungszentrum of Karlsruhe — We consider the out-of-equilibrium tunneling density-of-states for a two-dimensional diffusive film. Starting from a Keldysh FLorida, YUVAL GEFEN, Weizmann Institute of Science, ALEXANDER MIRLIN, University and Forschungszentrum of Karlsruhe — We consider the out-of- thermal equilibrium density-of-states for a two-dimensional diffusive film. Starting from a Keldysh

11:39AM V10.00003 Discrete breathers in Nonlinear Schrödinger hypercubic lattices with arbitrary power nonlinearity, JEROME DORIGNAC, JUN ZHOU, DAVID K. CAMPBELL, Boston University — We study two specific features of onsite breathers in Nonlinear Schrödinger systems on $d$-dimensional cubic lattices with arbitrary power nonlinearity: their wave functions and energies close to the anti-contiuum limit (small hopping limits) and their excitation thresholds. Exact results are compared to the predictions of the exponential ansatz (EA) and to the solution of the single nonlinear impurity model (SNI), where all nonlinearities of the lattice but the central one, where the breather is located, have been removed. The excitation thresholds predicted by the SNI solution are shown to be in excellent agreement with the exact results but cannot be obtained analytically except in 1D. We show that an EA approach to the SNI problem provides an approximate analytical solution that is asymptotically exact as the nonlinearity tends to infinity. We also prove a conjecture by Bustamante and Molina [Phys. Rev. B 62, 15287 (2000)] that the limiting value of the bound state energy of the SNI model is universal when the nonlinearity tends to infinity.
11:51AM V10.00004 Numerical renormalization group study of a dissipative quantum dot
M.T. GLOSSOP, K. INGERSENT, U. Florida — We study the quantum phase transition (QPT) induced by dissipation in a quantum dot device at the degeneracy point. We employ a Bose-Fermi numerical renormalization group approach [1] to study the simplest case of a spinless resonant-level model that couples the charge density on the dot to a dissipative bosonic bath with density of states \( B(\omega) \propto \omega^s \). In anticipation of future experiments [2] and to assess further the validity of theoretical techniques in this rapidly developing area, we take the conduction-electron leads to have a pseudogap density of states: \( \rho(\omega) \propto |\omega|^s \), as considered in a very recent perturbative renormalization group study [3]. We establish the conditions on \( r \) and \( s \) such that a QPT arises with increasing dissipation strength — from a delocalized phase, where resonant tunneling leads to large charge fluctuations on the dot, to a localized phase where such fluctuations are frozen. We present results for the single-particle spectrum and the response of the system to a local electric field, extracting critical exponents that depend in general on \( r \) and \( s \) and obey hyperscaling relations. We make full comparison with results of [3] where appropriate. Supported by NSF Grant DMR-0312939. [1] M. T. Glossop and K. Ingersent, PRL 95, 067202 (2005); PRB (2006). [2] L. G. G. V. Dias da Silva, N. P. Sandler, K. Ingersent, and S. E. Ulloa, PRL 97, 096603 (2006). [3] C.-H. Chung, M. Kircán, L. Fritz, and M. Vojta (2006).

12:03PM V10.00005 Anomalous Conductance Quantization in Side-Gated InAs Quantum Point Contacts
SAYDUR RAHMAN, University of Cincinnati, Cincinnati, Ohio 45221, STEVEN HERBERT, Xavier University, Cincinnati, Cincinnati, Ohio 45207, RICHARD NEWROCK, PHILIPPE DEBRAY, University of Cincinnati, Cincinnati, Ohio 45221 — Conductance measurements as function of Fermi energy of InAs quantum point contacts created by side gating on InAs/InAlAs quantum-well structure exhibit a distinct plateau at \( e^2/h \) and a less distinct one at \( 2e^2/h \). Applied magnetic field has little or no influence on the conductance quantization pattern. We believe the conductance plateau at \( e^2/h \) indicates a spin contribution of \( h/e^2 \) to the resistance of the one-dimensional channel when the electron density is low and the electron-electron interaction is strong. This can be understood in the framework of the recently proposed spin-incoherent Luttinger liquid (SILL) state that is considered to exist when \( J < c T < E_F \), where \( J \) is the spin exchange constant and \( E_F \) the Fermi energy. In the SILL regime, the spin excitations are reflected back to the leads reducing the conductance of the quantum wire to \( e^2/h \). At higher Fermi energy, when the electron density is higher, the spin contribution to resistance vanishes and the conductance takes the well-known quantized value of \( 2e^2/h \).

This work is supported by the National Science Foundation under grant DMR-0244489.

12:15PM V10.00006 Phase-ordering dynamics in itinerant quantum ferromagnets
R. SAHA, Dept. of Physics, University of Oregon, Eugene, OR 97403 and Dept. of Physics, University of Maryland, College Park, MD 20742, D. BELITZ, Dept. of Physics, University of Oregon, Eugene, OR 97403, T. R. KIRKPATRICK, Dept. of Physics, University of Maryland, College Park, MD 20742 — Phase ordering following a rapid quench from the disordered phase to the ordered phase occurs via growth of domains that arise from spontaneous fluctuations. The linear size \( L \) of these domains grow as a power law function of time for late times: \( L(t) \propto t^1/2 \), with \( z \) a dynamical exponent [1]. Until now this description of phase ordering dynamics has been applied to classical systems only. We apply this theory to describe domain growth in both clean and dirty itinerant quantum ferromagnets. The fluctuation effects that invalidate Hertz’s theory of the quantum phase transition [2] also affect the phase ordering. For a quench into the ordered phase a transient regime appears, where the dynamical exponent differs from the classical case, and for asymptotically long times the prefactor of the growth law has an anomalous magnetization dependence [3]. A quench to the quantum critical point results in a growth law which is not a power-law function of time. [1] A.J. Bray, Adv. in Phys. 43, 357 (1994). [2] D. Belitz, T. R. Kirkpatrick, and T. Vojta, Rev. Mod. Phys. 77, 579 (2005). [3] D. Belitz, T. R. Kirkpatrick, and Ronoojoy Saha, cond-mat/0610605.

12:27PM V10.00007 Universal non-linear conductivity near to an itinerant-electron quantum critical point
PATRICK HOGAN, ANDREW GREEN, University of St Andrews — Quantum critical systems display universal, power-law temperature dependence in their response functions. These universal power-laws provide an experimental window upon quantum criticality. Concentrating upon conductivity in itinerant-electron systems near a magnetic quantum critical point, we show that universal power-law dependence upon temperature is reflected in a universal non-linear conductivity; when a strong electric field is applied, the resulting current has a universal power-law dependence upon the applied electric field. For a system with thermal equilibrium resistivity proportional to \( T^\alpha \), we find a non-linear resistivity proportional to \( E^{\alpha/(1+\alpha)} \). This provides a new experimental handle upon the physics of itinerant-electron quantum critical points.

This work was supported by the Royal Society and the EPSRC.

12:39PM V10.00008 Quantum critical behavior in itinerant electron systems: Eliashberg theory and instability of a ferromagnetic quantum-critical point
JEROME RECH, Argonne National Laboratory, IL, CATHERINE PEPIN, SPHT CEA Saclay, France, ANDREY CHUBUKOV, University of Wisconsin-Madison, WI — We consider the problem of fermions interacting with gapless long-wavelength collective bosonic modes. The theory describes, among other cases, a ferromagnetic quantum-critical point (QCP). We construct a controllable expansion at the QCP in two steps: we first create a new, non Fermi-liquid “zero-order” Eliashberg-type theory, and then demonstrate that the residual interaction effects are small, provided we meet two conditions on the parameters of the system. For an \( SU(2) \) symmetric ferromagnetic QCP, we find that the Eliashberg theory itself includes a set of singular renormalizations which can be understood as a consequence of an effective long-range dynamic interaction between quasi-particles, generated by the Landau damping term. These singular renormalizations give rise to a negative non-analytic \( q^{1/2} \) correction to the static susceptibility, and destroy a ferromagnetic QCP. We demonstrate that this effect can be understood in the framework of the \( \phi^4 \) theory of quantum-criticality, and show that it is specific to the \( SU(2) \) symmetric case.

12:51PM V10.00009 Verification of universality in strong critical adsorption with three techniques
MATTHEW BROWN, BRUCE LAW, Kansas State University, LYLE MARSCHAND, LAURENCE LURIO, Northern Illinois University, SERIF URAN, Pittsburg State University — Fischer and de Gennes [C. R. Acad. Sci., Ser. B 287, 207 (1978)] suggested that for a mixture which was critical with respect to the demixing phase transition an interfacial adsorption profile would exhibit universal (system independent) scaling behavior. Carpenter et al. [Phys. Rev. E 61, 532 (2000) and references therein] verified this theory with a model which described ellipsometry data previously taken from several critical binary liquid mixtures. Until recently most of these data were not verified with any other experimental techniques. We describe a successful effort to verify Carpenter’s model with data from a neutron reflectometry study of a critical D2O + 3-methylpyridine mixture, as well as an analysis of data from both ellipsometry and x-ray reflectometry from a critical mixture of dodecane + tetrabromoethane.

PACS numbers DMR-0603144, 68.35.Rh, 68.43.-h, 64.60.Fr
1:03PM V10.00010 Critical Behavior Near the Ferromagnetic Transition in Nanostructured Gadolinium1, PAUL SHAND, JUSTIN BOHNET, University of Northern Iowa, JARED GOERTZEN, JEFFREY SHIELD, GEOFFREY SHELBURNE, DAVID SCHMITTER, DIANDRA LESLIE-PELEYCKY, University of Nebraska-Lincoln — ac susceptibility and dc magnetization have been measured near the ferromagnetic transition in melt-spun nanostructured Gd. Effective critical exponents and the critical temperature were extracted using modified Arrott plots. The values obtained were $\beta_{eff} = 0.415 \pm 0.005$, $\gamma_{eff} = 1.36 \pm 0.04$, $\delta_{eff} = 4.24 \pm 0.02$, and $T_C = 290.0 \pm 0.1 K$. These exponent values satisfy the scaling relation $\beta \delta = (\beta+\gamma)^2$. The experimental exponent values are also close to those for a short-range 3D Heisenberg ferromagnet; however, there is a systematic shift toward mean-field values. Such a shift has been previously seen in amorphous ferromagnets and is likely due to the presence of longer-ranged interactions, especially in Gd-based alloys. The critical exponents for nanostructured Gd are closer to the short-range 3D Heisenberg exponents than are those for amorphous Gd$_{70}$Co$_{20}$ and Gd$_{80}$Au$_{20}$. This suggests that the dominant Gd-Gd interactions are shorter-ranged in nanostructured Gd than in the amorphous alloys.

1Supported by NSF Grant Nos. DMR-0504177 and DMR-0504706

1:15PM V10.00011 Spin-orbit coupling triggered Mott insulator Sr$_5$IrO$_4$1, BUM JOON KIM, HOSJUB JIN, SOON JAE MOON, JAE-YOUNG KIM, CHOON SHIK LEEM, JAEJUN YU, TAE-WON NOH, CHANGYOUNG KIM, SE-JUNG OH, JAE-HOON PARK, GANG CAO — Electronic structures of 5d transition-metal oxide (TMO) Sr$_5$IrO$_4$ are investigated by angle-resolved photoemission spectroscopy and density-functional electronic structure calculations. The insulating nature of this compound and its measured valence band symmetry are correctly accounted for by the calculation only when both spin-orbit coupling and electronic correlation effects are included. It is shown that the spin-orbit coupling plays a crucial role in stabilizing the Mott-insulating ground state, which is unexpected in a compound with extended 5d valence band. The spin-orbit coupling leads to symmetry-split-off bands near the Fermi level which are large enough to be gapped by the Coulomb repulsion of moderate strength. This results in a conduction band as narrow as $\sim 0.5$ eV, defying its general character expected for 5d TMO. Our finding marks an establishment of a new type of Mott insulator and suggests possibility of novel Mott-derived phenomena in 5d based materials.

1:27PM V10.00012 Spin-orbit coupling in quasiperiodic systems, CARLOS WEXLER, University of Missouri and Institute of Solid State Physics, University of Tokyo. DAIJIRO TOBE, MAHITO KOHMOTO, Institute of Solid State Physics, University of Tokyo — Electrons in incommensurate systems (e.g., electrons in a lattice in presence of a perpendicular magnetic field) have a rich behavior exemplified by the beautiful Hofstadter butterfly, a self-similar spectrum which is a multifractal Cantor set. We analyze the effect of spin-orbit coupling in this system which can be described by a generalization of Harper’s equation. We find that the added term significantly modifies the scaling laws and appears to induce a delocalization of the insulator.

1:39PM V10.00013 Influence of Boundary Conditions on the Critical Scaling of Finite Systems, BENJAMIN VOLLMAYR-Lucke, Bucknell University, ERIK LUIJSEN, University of Illinois — We investigate the influence of boundary conditions on the behavior of finite spin systems at criticality; in particular, a comparison is made between periodic boundary conditions and free boundary conditions. Via simulations, we find that the critical magnetization distribution of the short-range Ising model with free boundary conditions differs significantly from the periodic case. We also consider spin systems with long-range interactions $V \sim 1/r^{(d+n)}$ for $n \leq 2$ the upper critical dimension is $d_c = 2n$, which allows for accurate simulations for $d > d_c$. Systems using analytic results from Bériton and Zinn-Justin for periodic boundary conditions, and then utilizing the techniques developed by Rudnick, Gaspari, and Privman for free boundary conditions, we obtain explicit expressions for the scaling of the susceptibility and the shape of the magnetization and energy distributions at criticality. The numerical data exhibit excellent agreement with our analytic results, providing in most cases the first explicit test for these predictions.

1:51PM V10.00014 Measurement Noise Maximum as a Signature of a Phase Transition1, ZHI CHEN, CLARE YU, University of California, Irvine — Noise is ubiquitous and is being increasingly used as an experimental tool to probe condensed matter systems, but unfortunately, when studying phase transitions, the usefulness of the experimental results is diminished by the fact that little is known about what to expect in the noise spectra. We propose that an increase in the measurement noise can be used to signal the onset of a phase transition since noise arises from the fluctuations of microscopic entities which, in turn, play a key role in phase transitions. As an example, we study the noise in the 2D Ising model which undergoes a second order phase transition, and in the 5-state Potts model which undergoes a first order phase transition by using Monte Carlo simulations. We monitor these systems as the temperature drops below the critical temperature. At each temperature, after equilibration is established, we obtain the time series of quantities characterizing the properties of the system, i.e., the energy and magnetization per site for different size of systems. We apply different methods, monitor these systems as the temperature drops below the critical temperature. At each temperature, after equilibration is established, we obtain the time series of quantities characterizing the properties of the system, i.e., the energy and magnetization per site for different size of systems. We apply different methods, and then analyzing the techniques developed by Rudnick, Gaspari, and Privman for free boundary conditions, we obtain explicit expressions for the scaling of the susceptibility and the shape of the magnetization and energy distributions at criticality. The numerical data exhibit excellent agreement with our analytic results, providing in most cases the first explicit test for these predictions.

1Supported by DOE grant DE-FG02-04ER46107

Thursday, March 8, 2007 11:15AM - 2:03PM —
Session V23 DCMP: High Pressure VI Colorado Convention Center 110

11:15AM V23.00001 Potentially novel ultrahigh pressure form of ABX$_3$-type compounds1, KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, MSI and CEMS, University of Minnesota — By means of first-principles computations we have identified two new dynamically stable structures that are candidate ultra-high pressure forms of ABX$_3$-type compounds. To our knowledge, they have not been experimentally observed yet. They are produced by metastable pressure-induced transformations in $\textit{Pm} \overline{3} \textit{m}$ NaMgF$_3$, a post-perovskite phase. The first transition to a $\textit{Pm} \overline{3} \textit{m}$ structure is related to a soft phonon mode in post-perovskite. The second one is a regular enthalpically driven transition from $\textit{Pm} \overline{3} \textit{m}$ to a $\textit{P} \overline{4}_1 \textit{mmm}$ structure. In NaMgF$_3$, these phases are metastable with respect to the dissociation into CsCl-type NaF and cotunnite-type MgF$_3$. However, the $\textit{Pm} \overline{3} \textit{m}$ phase might be observed at low pressures. We have also identified a candidate post-perovskite material that prefers the $\textit{Pm} \overline{3} \textit{m}$ phase over the dissociation into AX- and BX$_2$-type solids.

1Research supported by NSF/EAR 013533, 0230319, and NSF/ITR 0428774 (VLab). Computations were performed at the Minnesota Supercomputing Institute.

11:27AM V23.00002 Reactive Molecular Dynamics Studies of Thermal Induced Chemical in TATB, TIMOTHY GERMANN, JASON QUENNEVILLE, Los Alamos National Laboratory — Equilibrium molecular dynamics (MD) simulation of high explosives can provide important information on their thermal decomposition by helping to characterize processes with timescales that are much longer than those attainable with non-equilibrium MD shock studies. A reactive force field is used with MD to probe the chemistry induced by intense heating (‘cook-off’) of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). The force field (ReaxFF) was developed by van Duin, Goddard and coworkers [1] at CalTech and has already shown promise in predicting the chemistry in small samples of RDX under either shock compression or intense heat. Large-system simulations are desired for TATB because of the high degree of carbon clustering expected in this material. We will show results of 800-particle simulations at several temperatures, and detail current capabilities for large-scale ($10^4 - 10^5$ atoms) systems carried out with the massively parallel GRASP MD software developed at Sandia National Lab. Finally, we will compare the reaction timescales with those of RDX and HMX. [1] A. C. T. Van Duin, et al, J. Phys. Chem. A, 1005, 9396 (2001).
11:39AM V23.00003 Long timescale dynamics of shocked nitromethane  . LAURENCE FRIED, EVAN REED, RIAD MANAA, Lawrence Livermore National Laboratory. KURT GLAESEMANN, JOHN JOANNOPoulos, Massachusetts Institute of Technology — We present the farthest ever glimpse behind the shock front in a chemically reactive molecular dynamics simulation by applying a multi-scale shock wave simulation technique to the study of chemical reactions in shocked nitromethane (CH3NO2) represented by the DFTB tightbinding method. Shock speeds from 5.5 km/s to 8 km/s are simulated for durations up to 0.8 ns demonstrating substantial computational savings compared with the non-equilibrium molecular dynamics (NEMD)/shock simulation approach. These simulations indicate that the reaction zone in detonating nitromethane is greater than 0.3 μm in length. Ionic species are found to be prevalent in the early reactions of shocked nitromethane. Results are consistent with available experimental data. As a validation of our multiscale approach, we compare spatial wave profiles computed with the multiscale technique to profiles computed using the NEMD approach.

11:51AM V23.00004 Shear strain induced structural and electronic modifications of the energetic molecular crystal 1,1-diamino-2,2-dinitroethylen e1 . SERGEY RASHKEEev, Idaho National Laboratory, MALIA KURLJA, National Science Foundation — First-principles calculations of the structural and electronic properties of the deformed energetic molecular crystal 1,1-diamino-2,2-dinitroethylene (FOX-7) under shear-strain loading are presented. The reaction of the crystal to applied shear-strain loading is found to be highly anisotropic. When the external loading is removed, the relaxation of the system is mainly defined by stretching, bending, and rotations of the NO2 groups of neighboring molecules. In general, the deformed molecular crystal never relaxes to its initial, ideal crystalline FOX-7 structure. Instead, different planes remain shifted relative to each other on vectors, which are typically incommensurate with any translation vector of the ideal crystal. We also found that no metallization occurs under shear-strain loading. We suggest that the considered mechanisms of the shear-strain relaxation of the structural and electronic degrees of freedom are typical for layered anisotropic molecular crystals, and that they should significantly affect their chemical reactivity, conductivity, optical properties, and initiation of detonation in energetic materials.

— Physics — We report synchrotron FTIR and far infrared measurements on PETN, RDX, HMX and TATB at ambient temperature and high pressure, using YULGA, MICHAEL PRAVICA, UNLV - Physics, ZHENXIAN LIU, NSLS, Carnegie Institute of Washinton, OLIVER TSCHAUNER, MALCOLM NICOL, UNLV - Physics — We report synchrotron FTIR and far infrared measurements on PETN, RDX, HMX and TATB at ambient temperature and high pressure, using various media for pressurization of the samples. In all cases, we have carefully studied any phase transitions in the 0 - 15GPa pressure range and have cycled pressures to interrogate sample survivability and reproducibility of the phase sequences. For PETN, we used differering pressurizer media (Ar and KBr) and have found that the onset of a prior-reported phase transition around 5GPa varies with the different media, portending the importance of shear stress in inducing some or all of this phase transitions.

12:03PM V23.00005 An Infrared Study of Secondary Explosives under High Pressure.1 . BRIAN YULGA, MICHAEL PRAVICA, UNLV - Physics, ZHENXIAN LIU, NSLS, Carnegie Institute of Washinton, OLIVER TSCHAUNER, MALCOLM NICOL, UNLV - Physics — We report synchrotron FTIR and far infrared measurements on PETN, RDX, HMX and TATB at ambient temperature and high pressure, using various media for pressurization of the samples. In all cases, we have carefully studied any phase transitions in the 0 - 15GPa pressure range and have cycled pressures to interrogate sample survivability and reproducibility of the phase sequences. For PETN, we used differering pressurizer media (Ar and KBr) and have found that the onset of a prior-reported phase transition around 5GPa varies with the different media, portending the importance of shear stress in inducing some or all of this phase transitions.

We gratefully acknowledge support from the UNLV/ARL SOldier FERST program as well as partial support from the DOD MURI program. We gratefully acknowledge the support from the DOE Cooperative Agreement No. DE-FC08-01NV14049 with UNLV.

12:15PM V23.00006 Vibrational spectra of solid HNFX (C6H8F8N8O8): Experiments and theory1 . MALCOLM NICOL, CEDRIC GOBIN, EUNJA KIM, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, NV 89154 — Assignment of the vibrational spectra of molecular solids such as HNFX is very complex. We have made a combined experimental and theoretical study of the vibrational spectra of solid HNFX. Crystalline HNFX consists of unit cell with 9 HNFX molecules in C1 symmetry. Vibrational modes were calculated by using the PCFF force field method and were directly compared to measured IR and Raman spectra. A complimentary calculation for molecular HNFX allows us to identify the intramolecular motions measured in experiments. Intermolecular motion by F–H bonds between HNFX molecules will be discussed in this talk.

12:27PM V23.00007 High Pressure Behavior in Hydrated Metal Hexafluorosilicates M(H2O)6SiF6 , ALICE ACATRINEI, MONIKA HARTL, LUKE DAEMEN, JIANZHONG ZHANG, Los Alamos National Laboratory, LANSC- LC, YUSHENG ZHAO, Los Alamos National Laboratory — The octahedral (6-fold) coordination is highly unusual in Si chemistry, making hexafluorosilicates (HFS) interesting from a structural standpoint. It has been observed that Si coordinates to O octahedrally at extremely high pressures deep in the Earth mantle, but no compound possessing this property is known to be thermodynamically stable at ambient conditions. We suggest that HFS could act as surrogate materials to study Si in this coordination state in hydrated materials. Transition metal HFS exhibit a variety of structural transitions and magnetic properties changes when pressure is applied. Some structural phases and phase transitions exhibited by some compounds at ambient pressure can occur in other compounds at high pressure only. We examined the behavior of Zn(II) as well as Cd(II) and Hg(II) HFS hexafluorides as a function of pressure and temperature, and their possible role in understanding structural phase transitions in HFS. Measurements were performed between 0-18 GPa at room temperature.

12:39PM V23.00008 On the High-Pressure Behavior of Titanium Hydride . PATRICIA E. KALITA, Department of Physics,University of Nevada Las Vegas, NV, USA, STANISLAS SINOGEIKIN, Geophysical Lab, Carnegie Institution of Washington, Washington DC, USA, KRISTINA E. LIPINSKA-KALITA, Department of Chemistry, University of Nevada Las Vegas, NV, USA, THOMAS HARTMANN, Harry Reid Center of Environ. Studies, Las Vegas, NV, USA, ANDREW CORNELIUS, Department of Physics,University of Nevada Las Vegas, NV, USA — Hydrogen storage research has recently invested a great deal of effort towards investigations of metal hydrides. Although titanium hydride is not the ideal candidate for storing hydrogen, Ti hydrides can act as active species to catalyze the reversible dehydrogenation of other hydrides and carbon nanotubes. In addition the basic science interest of this project lies in investigating the structural and magnetic properties of this material. In the present study, we show that hydrogen storage in high-pressure angle-dispersive and energy dispersive synchrotron x-ray diffraction studies of titanium hydride. We investigate the effects of hydrostatic and non-hydrostatic conditions. We also show the results of structural refinements as well as the bulk modulus of TiH2. To the best of our knowledge, this work is the first attempt to measure the equation of state of TiH2 using synchrotron x-ray diffraction and diamond anvil cells.

12:51PM V23.00009 Pressure tuned phonon mode splitting in magnetic frustrated spinel ZnCr2O4 , TAO ZHOU, New Jersey Institute of Technology, ZHENXIAN LIU, Brookhaven National Lab, CHENGLIN ZHANG, SANG-WOOK CHEONG, Physics Department, Rutgers University — ZnCr2O4 has cubic spinel structure. Below 390 K, the geometrically frustrated magnet enters a paramagnetic state. Below 12.5 K, it undergoes a first-order phase transitions, resulting into an antiferromagnetic order and a structural distortion simultaneously. An IR-active phonon related to the Cr4+ ion’s motion undergoes a splitting at 12.5 K. This transition is explained as a spin-Peierls like transition. However, the exact cause and effect in such a transition is not clear. Is it because the lattice undergoes transition first, spin just follows, or is it spins’ interaction that forces the lattice to undergo changes? Pressure can provide a crucial service in clarifying this issue, since pressure can change spin and lattice interactions in different ways, it can differentiate these two scenarios. We have measured the infrared absorption spectra of ZnCr2O4 under pressure. Our data shows that Tc, at which the spin-Peierls like transition occurs and the phonon at about 370 cm−1 starts to show the splitting, increases from its ambient pressure value of 12.5 K to about 15.8 K at 1 GPa. This provides an important clue for the exact nature of this transition.
1:03PM V23.00010 Optical properties of CdSe semiconductor nanocrystals under high pressures. CHI-TSU YUAN, WU-CHING CHOU, DER-SAN CHUU, Department of Electrophysics, National Chiao-Tung University, Hsinchu 300, Taiwan — In general, the physical properties of semiconductor nanocrystals are different from the bulk materials. CdSe nanoparticles are attracted much attention due to excellent fluorescence properties for potential applications in biological labels.1 In particular, the emission colors can be tuned to cover whole visible range by changing particle size with the same chemical composition. On the other hand, high pressure technique is another tool to tune the electronic states of crystalline materials. Incorporated colloidal QDs under high pressure environment can provide valuable information to study the electronic and vibrational states of nanometer size materials. In this study, the electronic and vibrational states of colloidal core/shell CdSe/ZnS quantum dots are studied at room temperatures by using high pressure optical measurements. Pressure dependent quadratic lattice behavior can be observed clearly from photoluminescence (PL) and Raman spectra up to ~7 GPa. This quadratic relationship is consistent with theoretical prediction. The average pressure coefficients for PL and Raman measurements, as well as deformation potential are 32 meV/GPa, 4.2 cm$^{-1}$/GPa and -1.69 eV, respectively. [1] M. Jr Bruchez, M. Moronne, P. Gin, S. Weiss, and A. P. Alivisatos, Science 281, 2013 (1998).


1:27PM V23.00012 Pressure dependance of the Curie temperature of TbNi2Mn, investigated using designer diamond anvils1. DAMON JACKSON, SCOTT MCCALL, SAMUEL WEIR, Lawrence Livermore National Laboratory, DAVEN, Louisiana State University, QIU WEI, YOGESH VOHRA, University of Alabama, Birmingham — TbNi2Mn is a cubic Laves structured material with a Curie temperature at ambient pressure of Tc = 151 K. The behavior of the Curie temperature has been investigated by AC magnetic susceptibility under both hydrostatic and non-hydrostatic conditions using designer diamonds up to 29 GPa, for which it was found to decrease at $dT_c/dP = -2.0$ K GPa$^{-1}$. However, non-hydrostatic conditions result in a flattening out of $T_c$ with pressure which is non-reservable.

1Work at LLNL was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory, under Contract W-7405-Eng-48.

1:39PM V23.00013 Spectroscopic evidence for pressure-induced metallization in solid silane1. XIAO-JIA CHEN, VIKTOR V. STRUZHKIN, ALEXANDER GONCHAROV, YANG SONG, ZHEN-XIAN LIU, HO-KWANG MAO, RUSSELL J. HEMLEY, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015 — Infrared reflectance measurements on solid silane SiH4 have been performed under pressure up to 70 GPa at room temperature. After passing through three phase transformations, solid SiH4 is already black at 30 GPa. At high pressures around 60 GPa, the infrared reflectance spectra exhibit a Drude metallic behavior, signaling the pressure-induced metallization in solid silane. Angle-dispersive powder x-ray diffraction studies reveal that a structural transition is accompanying the silane transition to the metallic state.

1The work was supported by the DOE Grant DEFG02-02ER4595, and CDAC Grant DEFC03-03NA00144.

1:51PM V23.00014 Search for superconductivity in LiBC at high pressure1. AMY LAZICKI, Lawrence Livermore National Laboratory, University of California, Davis, CHOONG-SHIK YOO, HYUNCHAE CYNN, WILLIAM J. EVANS, Lawrence Livermore National Laboratory, WARREN E. PICKETT, JUSTIN OLAMIT, KAI LIU, University of California, Davis, Y. OHISHI, SPring-8/JASRI, Hyogo 679-5198, Japan — Lithium borocarbide, which is a structural and electrical analog to high-Tc superconductor MgB2, remains insulating at ambient conditions due to atomic alternation in the crystal structure. We investigated experimentally and theoretically the properties of this material under pressure, including structural and bonding anisotropy and the possibility of metallization and superconductivity under high pressure. It is found to remain stable up to 60 GPa with no crystal structure change and without a previously reported lattice parameter anomaly. In this crystal structure, metalization is not predicted to occur until at least 345 GPa, at which pressure the electronic bands responsible for superconductivity in MgB2 remain unoccupied in LiBC, ruling out the possibility of a new MgB2-like high pressure superconductor.

1This work has been supported by the LDRD(04ERD020) and SEGRF programs at LLNL, University of California, under DOE Grant No. W7405-ENG-48, by the SSAAP (DE-FG01-06NA2620) and by the Alfred P. Sloan Foundation.

Thursday, March 8, 2007 11:15AM - 2:03PM – Session V42 DCMP: Metal Oxides: Growth, Structure, Interfaces Colorado Convention Center 505

11:15AM V42.00001 Characterization of Epitaxial Ag2-xO Thin Films Grown on Sapphire. S.B. RIVERS, Rhode Island College, G. BERNARDT, M.W. WRIGHT, D.J. FRANKEL, M.M. STEEVES, R.J. LAD, University of Maine — We have grown silver oxide films with a range of stoichiometry near Ag2O by x-beam evaporation of silver in an oxygen electron cyclotron resonance (ECR) plasma. Films were deposited on r-cut sapphire substrates. A quartz crystal oscillator was used to monitor the film growth and to determine ECR oxygen flux by examining the rate of oxygen uptake on a silver film. This information was used to select the silver rate (0.1 or 1.0 ˚A/s) and the oxygen flow rate (from 2 to 10 sccm). XRD and RHEED analysis reveals films grew with one-dimensional \langle111\rangle epitaxy, true three-dimensional \langle002\rangle epitaxy, or a mixed phase depending on the deposition conditions. XRD and XPS shows the composition varies with deposition conditions and can be a mixture of AgO and Ag2O. UV-vis spectroscopy shows that the films have a single absorption edge between 3.1 and 3.5 eV. Optical transmission from 500 to 700 nm is between 70 and 80%. Four-point der van Pauw conductivity and Hall effect measurements indicate that the Ag2-xO films are p-type with a conductivity on the order of $3 \times 10^{-3}$ $\Omega^{-1}$ cm$^{-1}$.
11:27AM V42.00002 Ultrathin CoO (100) films on Fe2O3 (100): a photoemission study1, HUI-QIONG WANG*, ERIC I. ALTMAN**, VICTOR E. HENRICH*, Departments of Applied Physics* and Chemical Engineering**, Center for Research on Interface Structures and Phenomena (CRISP), Yale University — Using molecular beam epitaxy (MBE), 1 to 20 monolayer (ML) thick CoO (100) films were grown monolayer by monolayer on Fe2O3 (100) substrates. Auger measurements as a function of CoO film thickness indicated a layer-by-layer growth mode. Ultraviolet photoelectron spectroscopy (UPS) was used to monitor the evolution of the thin film electronic properties. To avoid oxidizing the Fe2O3 surface, Co was deposited in UHV and then oxidized for each monolayer. By comparing UPS spectra taken before and after oxidation of the Co, the separate contributions of Co and oxygen to the valence band electronic structure could be identified. Very thin (e.g., 1 – 3 ML) films exhibit valence band structures very different from those of bulk CoO. The interfacial electronic states were analyzed by comparing measured and model UPS spectra.

1This research is partially supported by U.S. Department of Energy Grant No. DE-FG02-00ER45844, NSF Equipment Grant No. DMR-0075824, and NSF Grant MRSEC DMR-0520495.

11:39AM V42.00003 Biaxial Texture Evolution in Ion-Beam Assisted Deposition of MgO . VLADIMIR MATIAS, MPA-STM, Los Alamos National Laboratory — We examine the evolution of biaxial crystalline texture during ion-beam assisted deposition (IBAD) of MgO using reflection high-energy electron diffraction, in situ ion scattering, and x-ray diffraction. The IBAD-MgO templates on metal tape are used for second generation high-temperature superconductors, also known as coated conductors. For MgO and some other materials with a rock salt crystalline structure, IBAD texturing can be achieved within the first few nanometers of deposited material. We find that the texture development is very sensitive to the nucleation surface conditions, both chemical species and surface morphology. In the best cases an in-plane texture of 2 degrees and an out-of-plane texture of 1 degree are attainable in a homoepitaxial MgO layer. We are utilizing a methodology of presenting data in terms of IBAD texture contour plots where we collect data as a function of ion-to-molecule ratios and film thickness. The striking conclusion from the data is that the texture development for different ion-to-molecule ratios can be scaled with the cumulative ion damage normalized to deposited MgO material. We discuss the results in terms of possible mechanisms for IBAD-MgO biaxial texturing and relationship to other IBAD texturing processes. This work is supported by the Department of Energy Office of Electricity Delivery & Energy Reliability.

11:51AM V42.00004 Phase diagram for the Ni/Al2O3 interface and relationships to adhesion . XIAO-GANG WANG, JOHN SMITH, Delphi Research Labs, Shelby Township, Michigan 48315, USA — First-principles calculations conducted over a broad range of atomic configurations have been used to determine the phase diagram and work of separation for Ni/Al2O3 interfaces[1]. Seven interfacial phases have been identified. The results reveal that the strongest (O-rich) phases derive their strength from ionic Ni-O bonds across the interface, reminiscent of NiO. The range of atomic configurations have been used to determine the phase diagram and work of separation for Ni/Al2O3 systems.

12:03PM V42.00005 Interplay between structure and electronic properties in metal-oxide interfaces . MATIAS NUNEZ, MARCO BUONGIORNO NARDELLI1, Department of Physics, North Carolina State University, Raleigh, NC 27695, USA — Using first principles calculations we have investigated a broad spectrum of metal-insulator interfaces, including crystalline oxides and ferroelectrics. In our study we have focussed on the role of the interface phase in determining the properties of the composite system and, in particular, the relation between interface structure, charge transfer at the interface, and the associated interfacial dipole. For crystalline oxides such as BaTiO3, our results demonstrate the possibility of tuning the Schottky barrier height by manipulating the interface phase. [1] Ferroelectric materials, such as BaTiO3, have been analyzed the interplay between the interface phase, the thickness of the ferroelectric layer and the residual polarization of the thin film. The polarization of the ferroelectric has been computed using modern theory of polarization via the displacements of the centers of the Wannier functions associated with the system. [1] M. Nunez and M. Buongiorno Nardelli, Phys. Rev. B 73, 235422 (2006).

12:15PM V42.00006 Morphology of cerium oxide surfaces in an oxidizing environment: a first-principles investigation . MARCO FRONZI, ALOYSIUS SOON, CATHARINE STAMPFL, School of Physics, University of Sydney, Australia, BERNARD DELLEY, Paul-Shererr Institute, ENRICO TRAVERSA, University of Tor Vergata, Rome — A good understanding of the stability and chemistry of CeO2 surfaces is crucial for a better designing of solid oxide fuel cells. As the first step, we use DFT [1] to study the structural and electronic ground state properties of bulk CeO2, various surface termination of the low-index surface of CeO2 are then investigated, namely the stoichiometric, metal- and oxygen-rich terminations, and defected surfaces. Using the concept of “ab initio atomistic thermodynamics” [2], we calculate the surface free energy phase diagram. This allows us to identify and predict stable, and potentially catalytically important, structures. There is an evidence that suggests an interesting morphological change in the surface structures with varying oxygen concentration. Reaction pathways for methane oxidation on low energy cerium oxide surfaces are being investigated and will be reported.


12:27PM V42.00007 Stabilization mechanisms of polar ZnO surfaces revisited . SHENGBAI ZHANG, National Renewable Energy Laboratory, MAO-HUA DU, STEVEN ERWIN, Naval Research Laboratory, JOHN NORTHUP, Palo Alto Research Center — The polar (0001) surfaces of ZnO exhibit a variety of different morphologies. The mechanisms underlying this diversity have not been definitively identified. Here we evaluate the role of several possible candidates. We show that electrosstatics does not play a significant role. Instead, we argue that surface morphology is determined by a competition between two other mechanisms. The first is the electron counting rule, which leads to semiconducting surfaces. The second arises from the large cohesive energy of ionic crystals such as ZnO, which tends to preserve the surface stoichiometry at its bulk value, leading to metallic surfaces. First-principles calculations show a crossover in the relative stability of semiconducting and metallic surfaces as the chemical potential of oxygen is varied. This behavior accounts for the many observed surface morphologies on ZnO(0001), including triangular islands and pits.

12:39PM V42.00008 Crystalline Metal Oxide Nanoparticle Films for Renewable Energy Technologies . ANNE DILLON, SE-HEE LEE, ROHIT DESHPANDE, PHILIP PARILLA, KIM JONES, HARV MAHAN, NREL — Hot-wire chemical vapor deposition (HWCVD) has been employed as a scalable method for the deposition of crystalline tungsten oxide nanoparticles and nanorods. Under optimal synthesis conditions, only crystalline WO3 nanoparticles with a smallest dimension of ~ 10 - 50 nm are observed with extensive transmission electron microscopy (TEM) analyses. X-ray diffraction (XRD), Raman spectroscopy and electron diffraction confirm that the crystalline phases of the nanostructures may be tuned by varying the synthesis conditions such that a single phase is obtained. HWCVD has also been employed to produce crystalline molybdenum oxide nanoparticles at high density. TEM analyses show that the smallest dimension of these nanostructures is ~ 5 – 30 nm. XRD and Raman analyses reveal that the materials are highly crystalline and consist of Mo2O5 and MoO3 phases. It is also possible to fabricate large area porous films of either the tungsten or molybdenum oxide nanoparticles using a novel electrophoresis deposition technique. Furthermore, WO3 nanoparticle films have led to profound advancement in state-of-the-art electrochromic technologies, and MoO3 films are promising for new lithium-ion batteries.
Fermi edge suggest metallic behavior of the Au rows. The bonding to the substrate is predominantly covalent. Intra- and inter-chain spacings are determined coupling near the Neel temperature.

Our predictions relate readily observable quantities and allow for a parameter-free comparison with experiments.

square “level velocity” (the derivative of the energy with respect to magnetic field) calculated at magnetic fields larger than a characteristic correlation field.

relations assume that the electron dynamics in the grain is chaotic. The expressions we provide connect the second moment of the $g$ factors and discrete energy level velocities in nanoparticles where spin-orbit coupling is present. These relations assume that the electron dynamics in the grain is chaotic. The expressions we provide connect the second moment of the $g$ factor to the root-mean square “level velocity” (the derivative of the energy with respect to magnetic field) calculated at magnetic fields larger than a characteristic correlation field. Our predictions relate readily observable quantities and allow for a parameter-free comparison with experiments.

1:03PM V42.00010 The Onset of Ordered Vacancy Configurations on the TiO$_2$ (110) Surface. SCOTT J. THOMPSON, STEVEN P. LEWIS, University of Georgia — The (110) surface of TiO$_2$ is a prototypical metal-oxide surface system that has numerous important industrial applications relating to solar energy, gas sensors, and the decomposition of harmful organic compounds. Extensive experimental and theoretical studies have shown that the most common surface defects, bridging O vacancies, play an important role in the desired oxidation processes of this model photocatalyst. Additionally, experimentally observed surfaces have shown the tendency for these defects to arrange themselves in both isolated and highly ordered configurations at low and high vacancy concentrations, respectively. Through Monte Carlo simulations of a converged cluster-expansion model parameterized by density functional calculations, we have observed the onset of multiple ordered configurations of bridging oxygen vacancies at different concentrations. In this talk, we will present our results that show two long-ranged ordered configurations over a relatively wide range of chemical potentials in addition to two semi-ordered configurations, all of which are in good qualitative agreement with experimental and theoretical results.

1:15PM V42.00011 One-dimensional Au chains on TiO$_2$(110). ADAM KIEJNA, TOMASZ PABSIAK, University of Wroclaw, Poland — One-dimensional (1D) Au chains on the 1×2 missing row (mr) defected, and the added row (ar) reconstructed, TiO$_2$(110) surfaces are calculated from first principles. Single, dimer, and triple Au rows were considered. The single Au row binds strongly to the mr (2.83 eV) but much weaker to the ar surface (1.56 eV). On the mr surface the bonding of Au is mainly to the Ti atoms below, and to the neighboring Au atoms. In the mr surface the binding energy is decreasing with the number of Au atoms per row, while in the ar surface converse is observed. Even for triple Au rows the binding per atom (2.42 eV) is by 0.17 eV stronger for the mr than for the ar, the latter being suggested as the most favored structure of the clean surface. Thus, Au forms on the 1×2 missing row TiO$_2$(110) surface strongly adsorbed 1D chains. The charge density distribution and the increased density of occupied states around the Fermi edge suggest metallic behavior of the Au rows. The bonding to the substrate is predominantly covalent. Intra- and inter-chain spacings are determined by the substrate periodicity. The large inter-chain distance (13 Å) on the more or less insulating substrate makes this system ideal for studies of 1D phenomena.

1:27PM V42.00012 Time Resolved Surface Diffuse Scattering During Oxide Growth. J.Z. TISCHLER, B.C. LARSON, GYULA ERES, C.M. ROULEAU, Oak Ridge National Laboratory, P. ZSCHACK, Advanced Photon Source — The time dependence of surface x-ray diffraction during pulsed laser deposition provides detailed information about transverse surface structure and interlayer transport during layer-by-layer growth. To investigate the nature of growth during homoeptaxy of SrTiO$_3$, we measured the time-dependent evolution of surface diffuse scattering around the specular crystal truncation rod during deposition from a single laser shot (0.1 monolayer/pulse) on a pristine surface of (001) SrTiO$_3$. We observed the nucleation of very small islands and measured the time dependence of ripening into larger structures for the temperature range of 600 to 760°C. We will relate these measurements to measurements of time-resolved diffuse scattering from multiple pulses during layer-by-layer growth and previous measurements of time-resolved truncation rod intensities.

12:51PM V42.00009 Nanostructured Molybdenum Oxides for Lithium-Ion Batteries. SE-HEE LEE, ROHIT DESHPANDE, PHIL PARILLA, KIM JONES, BOBBY TO, HARV MAHAN, ANNE DILLON, National Renewable Energy Laboratory — Lithium-ion batteries are the current power sources of choice for portable electronics. Although such batteries are commercially successful, they are not keeping pace with the rapid advances in computing technologies. Also, further improvement of performance and simultaneous reduction in cost is still in need. Here we report the synthesis and electrochemical performance of a novel molybdenum oxide nanoparticle anode that dramatically improves the capacity, energy density, and cycle life of rechargeable lithium-ion batteries. Molybdenum oxide nanotubes (HWCVD) technique and a recently developed electrophoresis technique is employed for the fabrication of porous nanoparticle anodes. Our material exhibits a high reversible capacity of ~600 mAh/g in the range 0.005-3.0 V with excellent cycling characteristics as well as high-rate capability. Both cycling stability and rate capability issues are addressed by employing these porous molybdenum oxide films that consist of nanoscale active particles. These materials will impact the next generations of rechargeable lithium batteries, not only for applications in consumer electronics, but also for clean energy storage and use in hybrid electric vehicles.

1:39PM V42.00013 Leakage current reduction and magneto-electric coupling studies in BiFeO$_3$ thin films. N.M. MURARI, ASHOK KUMAR, UPR, RAM S. KATIYAR, University of Puerto Rico — The sol-gel derived BiFeO$_3$ thin films were prepared on Pt/Si substrate with less than 20nm of interfacial layer of Ba$_{0.25}$Sr$_{0.75}$TiO$_3$ (BST). The XRD data revealed a single-phase compound having crystallite size of 25-50 nm. Surface morphology was characterized utilizing atomic force microscope and the surface roughness and the particle size were found to be reduced compared to BFO films grown without the BST sheet layer. Current voltage characteristic graphs indicated a significant reduction in leakage current of 2-3 orders of magnitude. Anomalies in the dielectric constant as a function of temperature were observed near the Neel temperature ~600K which are indicative of the so called magneto-electric coupling in this compounds. Tangent loss spectra as a function of temperature and frequencies indicated the dielectric relaxation near the Neel temperature. Micro Raman spectroscopy was carried out as a function of temperature shows the disappearance of normal modes in the range of 300-600 cm$^{-1}$ and there was a shift towards the low frequency side with increase in half width. The anomalies in Raman spectra also support the spin-phonon coupling near the Neel temperature.

1:51PM V42.00014 Ab initio Study of Metal Interfaces with HfO$_2$ and SiO$_2$: Work Function Modulation. BLANKA MAGYARI-KÖPE, YOSHIO NISHI, Electrical Engineering, Stanford University, CA, LUIGI COLOMBO, Texas Instruments Incorporated, Dallas, TX, KYEONGJAE CHO, Physics and Electrical Engineering, University of Texas, Dallas, TX — For the next generation of metal-oxide-semiconductor field-effect transistors (MOSFETs), the suitable metal candidate has to be identified. The choice of a specific metal electrode on high-k gate dielectric oxides is strongly influenced by the possible interface chemical reactions and defects. In this study, ab initio calculations are employed to investigate and analyze a number of possible interface structures between gate dielectric oxides, HfO$_2$ and SiO$_2$, and metal electrodes. The structural stability and electronic structure of the interfaces with implications to metal work functions are discussed. The work function of metals on oxides is significantly influenced by the interface configurations and by the particular bonding pattern at the interface. For work function modulation, model interface systems of metal bi-layers are constructed based on structural and compositional heterogeneity. It is found that a few atomic layers of the underlying metal shift the work function of bi-layers to that of underlying metal.

11:27AM V43.00002 Full counting statistics for a quantum nanoelectromechanical system. STEVEN BENNETT, AASHISH CLERK, McGill University — Experiments on nanoelectromechanical systems often involve the effects of a mechanical oscillator on the current noise of a mesoscopic conductor. Coupling to the oscillator induces correlations between tunneling electrons in the conductor, leading to signatures in the shot noise. To better characterize such correlations it is useful to consider full counting statistics (FCS), which describe the complete probability distribution of tunnelled charge. We study theoretically the FCS in a tunnel junction coupled to a nanomechanical oscillator. This system has been realized in experiment using an atomic point contact where one electrode is free to vibrate and it has been predicted that the oscillator dynamics leads to large signatures in the shot noise that cannot be explained classically. Thus motivated, we investigate the FCS using a reduced density matrix tracking the oscillator and the number of tunnelled electrons, for which we obtain an equation of Caldeira-Leggett form with additional terms due to tunneling.


11:39AM V43.00003 Ab Initio Calculations for the Surface Energy of Silver Nanoclusters1, BHARAT MEDASANI, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, New Mexico 88003, YOUNG HO PARK, Department of Mechanical Engineering, New Mexico State University, Las Cruces, New Mexico 88003 — We apply first principles computational methods to study the surface energy and the surface stress of silver nanoparticles. The structures, energies and lattice contractions of spherical Ag nanoclusters are calculated in the framework of density functional theory combined with the generalized gradient approximation. Our calculations predict the surface energies of Ag nanoclusters to be in the range of 1–2 J/m². These values are close to the bulk surface energy of silver, but are significantly lower than the recently reported value of 7.2 J/m² derived from the Kelvin equation for free Ag nanoparticles. From the lattice contraction and the nearest neighbor interatomic distance, we estimate the surface stress of the silver nanoclusters to be in the the range of 1–1.45 N/m. This result suggests that a liquid droplet model can be employed to evaluate the surface energy and the surface stress of Ag nanoparticles.

1Supported by NSF DMR-0505270, PRF 43409-G10, and NMSU CORC Mini-Grant.

11:51AM V43.00004 The structures and energetics of interacting ionic nanocrystals from atomistic simulations.1, PAUL TANGNEY, Molecular Foundry, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, Molecular Foundry, Lawrence Berkeley National Laboratory and Department of Physics, University of California at Berkeley — Self-assembled ordered aggregates of nanocrystals (NCs) of many different sizes, shapes and compositions have been synthesized in recent years. These “supercrystals” form a new class of material with potentially new and useful properties in which nanoparticles take the place of atoms as the fundamental building blocks of matter. However, at present neither the detailed structures of NCs themselves nor the interactions between them are well understood and it is not yet clear which forces are responsible for binding and ordering them in supercrystals. In this work, NCs of highly ionic materials are simulated using first principles molecular dynamics (MD) and MD based on accurate polarisable force-fields. Individual NCs and multiple NCs in close proximity are simulated and their structures and the electrostatic contributions to their energetics are studied in detail. From our understanding of NCs in this ionic limit we provide insight into the importance of electrostatic contributions to NC bonding in more covalent materials.

1Supported by DOE, BES, under Contract No. DE-AC0205CH11231.

12:03PM V43.00005 Fermi-edge singularity in a spin-incoherent Luttinger liquid1, GREGORY A. FIETE, California Institute of Technology — We theoretically investigate the Fermi edge singularity in a spin incoherent Luttinger liquid. Both cases of finite and infinite core hole mass are explored, as well as the effect of a static external magnetic field of arbitrary strength. For a finite mass core hole the absorption edge behaves as $(\omega - \omega_i)^\alpha$ for frequencies $\omega$ just above the threshold frequency $\omega_i$. The exponent $\alpha$ depends on the interaction parameter $g$ of the interacting one dimensional system, the electron-hole coupling, and is independent of the magnetic field strength, the momentum, and the mass of the excited core hole (in contrast to the spin coherent case). In the infinite mass limit, the spin incoherent problem can be mapped onto an equivalent problem in a spinless Luttinger liquid for which the logarithmic factor is absent, and backscattering from the core hole leads to a universal contribution to the exponent $\alpha$.

1cond-mat/0605101 (To appear in Phys. Rev. Lett.)

12:15PM V43.00006 Free Energy of a 1D Metal-Molecule Interface: C_{60}-Decorated Ag Islands2, T. J. STASEVICH, National Cancer Inst., NIH, C. TAO, E. D. WILLIAMS, T. L. EINSTEIN, U. Maryland, College Park — We study the structural and dynamical properties of one-dimensional metal–molecule interfaces by investigating Ag monolayer islands on Ag(111) decorated by C_{60}. At 300K bare Ag(111) islands have hexagonal equilibrium shapes. When C_{60} is deposited on the surface, it preferentially nucleates along island step edges, near the island corners, making them round. We tune coverage so that a single chain of C_{60} fully decorates the island, forming a closed ring, circular in shape. From a simple model for the C_{60} step decoration, we derive the decorated step free energy as a function of step angle, yielding the equilibrium shape of the decorated islands via the Wulff construction. By comparing the model to experiment, we estimate the Ag-C_{60} attraction. Using fast STM scanning, we also study the fluctuations of the C_{60} decorated islands. By fitting the time correlation function of the fluctuation component Fourier modes, we show the decorated step dynamics are consistent with attachment-detachment (AD) kinetics, in contrast to the step-edge diffusion of the bare island. Finally, from our analysis, we extract the decorated step free energy and estimate the C_{60}-C_{60} attraction.

2Supported by NSF MRSEC Grant DMR 05-20471

12:27PM V43.00007 Permanent polarization of small metallic particles, ANDREY SHYTOV, Brookhaven National Laboratory, MICHAEL PUSTILNIK, Georgia Institute of Technology — Electric charge density in a metal fluctuates on the spatial scale of the Fermi wavelength due to various types of disorder. These fluctuations are usually compensated in the bulk due to Coulomb interaction between electrons. However, a small metallic particle may have a non-vanishing static electric dipole moment, owing to uncompensated density fluctuations near the surface on the scale set by the screening length. We analyze these fluctuations statistically and find that the typical value of the dipole moment increases linearly with the particle size, and fluctuates strongly from particle to particle. Our results are applicable to small metallic clusters and nanocrystals.
12:39PM V43.00008 Tuning the Conductivity of Semiconductor Nanostructures by Dielectric Engineering. ANIRUDDHA KONAR, DEBDEEP JENA, University of Notre Dame — Electron transport properties in semiconductor nanoscale quantum structures grown by bottom-up techniques can be fundamentally different from those grown by epitaxial methods. Transport properties in 1D nanotubes and nanowires and 2D nanoscale thin films are strongly affected by carrier-impurity interactions mediated by the dielectric environment of the nanostructure. We show that by suitable dielectric engineering of this environment, electron mobility in 1D and 2D semiconductor nanostructures can be enhanced by 1-2 orders of magnitude. The enhancement takes place only when the smallest length scale of the nanostructure is less than the effective Bohr radius of the bulk semiconductor. The enhancement in mobility occurs predominantly due to a large damping of Coulombic scattering, which results in a reduction of electron scattering rates. When the dielectric constant of the environment is changed from 1 (air) to 100 (high-k oxide dielectric), the Coulomb scattering rate decreases from 700/ps to 4/ps for a 1D nanowire, and from 66/ps to 3/ps for a 2D sheet. When other scattering mechanisms such as surface roughness and phonon scattering are considered, we find that the total conductivity of the nanostructures can be enhanced by 1-2 orders of magnitude by coating them with high-k dielectrics.

12:51PM V43.00009 Dielectrophoretic alignment of VO$_2$ nanowires in device geometries. IRVING HERMAN, SARBAJIT BANERJEE, VLADIMIR BLAJOJEVIC, KELLEN PETERSEN, MANAV MALHOTRA, MICHAEL STEIGERWALD, LOUIS BRUS, Materials Research Corporation and the Engineering School of Columbia University. VO$_2$ nanowires have been characterized by a Mott metal—insulator phase transition at ~68 °C and has been widely studied for optical and electrical switching applications. However, nanostructured vanadium oxides have been challenging to fabricate and thus not much is known about their properties. Here, we present the AC dielectrophoretic alignment of hydrothermally grown VO$_2$ nanoribbons, ~40 nm in width and several micrometers in length, in device geometries. The alignment process has been studied as a function of the applied voltage and frequency, gap distance, and concentration of the VO$_2$ dispersion. VO$_2$ nanowires have also been precisely positioned in different device geometries, such as across deep trench structures. The electrodes have been designed based on electric-field simulations. The nanowire devices show gate dependence at room temperature. The temperature dependence of the transport properties has also been examined. This work has been supported primarily by the MRSEC Program of the National Science Foundation under Award Number DMR-0213574 and the New York State Office of Science, Technology and Academic Research (NYSTAR), and partially by the NSEC Program of the National Science Foundation under Award Number CHE-0641523.

1:03PM V43.00010 Universal behavior of self-dangling bonds in hydrogen-terminated Si, Ge, and Si/Ge nanowires.¹, RICARDO NUNES, Universidade Federal de Minas Gerais - UFMG, RICARDO KAGIMURA, HÉLIO CHACHAM, UFMG — We report an ab initio study of the electronic properties of surface dangling bond (SDB) states in hydrogen-terminated Si, Ge, and Si/Ge nanowires with diameters between 1 and 2 nm. We find that the charge transition levels $\epsilon(+/−)$ of SDB states are deep in the bandgap for Si wires, and shallow (near the valence band edge) for Ge wires. In both Si and Ge wires, the SDB states are localized. We also find that the SDB $\epsilon(+/−)$ levels behave as a “universal” energy reference level among Si, Ge, and Si/Ge wires within a precision of 0.1 eV. By computing the average between the electron affinity and ionization energy in the atom of several atoms from the III, IV and V columns, we conjecture that the universality is a periodic-table atomic property.

¹Acknowledge support from CNPq, FAPEMIG, and Instituto do Milênio de Nanotecnologia - MCT/Brazil

1:15PM V43.00011 Superlattice nanowires via double-sided heteroepitaxy on compliant ultrathin Si ribbons.¹, CLARK S. RITZ, University of Wisconsin, Madison, FRANK S. FLACK, MICHELLE M. ROBERTS, DOUGLAS M. DETERT, YU ZHANG, University of Utah, DONALD E. SAVAGE, PAUL G. EVANS, FENG LIU, University of Utah, MAX G. LAGALLY — We fabricate and characterize a novel type of Si/Ge superlattice nanowire. Such structures, traditionally created by VLS growth, have been of great interest for thermoelectric applications for some time. We have developed a creating superlattice-like system using strained SiGe epitaxial islands. We pattern free-standing Si nanowires made from ultrathin silicon-on-insulator (SOI) substrates and use them as a substrate for the Stranski-Krstanov growth of coherent 3D islands. Interaction between islands growing on the top and bottom surfaces causes them to order laterally. The periodic strain induced in the substrate by the ordered islands affects the electronic band structure in a periodic way. The discussion will cover the fabrication and electrical properties of these strain superlattice structures.

¹Supported by DOE and AFOSR.

1:27PM V43.00012 Ground-state properties of quantum rings with a few electrons, YASUHIRO SAIGA, DAI HIRASHIMA, Nagoya University, JUNKO USUKURA, Tokyo University of Science — Quantum dots occupy an important position not only in the field of basic science, but also in the field of nanotechnology. Among various shapes of dots, a ring structure is a particularly interesting nanostructure, because the diameter and the ring width can be separately changed. In this talk, we discuss the ground-state properties of one-dimensional quantum rings with a few electrons, which interact with each other in the form of 1/r-Coulomb repulsion. By using exact diagonalization, we find that for three electrons, the fully spin-polarized ground state is uniquely realized when the diameter of the ring is sufficiently large. In contrast, for four and five electrons, the fully polarized state never becomes the unique ground state, however large the diameter is. These results can be understood in terms of multiple-spin exchanges. We also show that a magnetic field applied perpendicular to the ring induces not only the persistent current but also the spin chirality.

1:39PM V43.00013 Quantum Impurities and Persistent Currents: Decoupling through Integrability, HANS-PETER ECKLE, Advanced Materials Science, University of Ulm, JOHAN NILSSON, Department of Physics, Boston University, HENRIK JOHANNESSEN, Department of Physics, Göteborg University — We consider the problem of a persistent current in a one-dimensional mesoscopic ring with the electrons coupled by a spin exchange to a magnetic impurity. We show that this problem can be mapped onto an integrable model with a quadratic dispersion (with the latter property allowing for an unambiguous definition of the persistent current). We have solved the model exactly by a Bethe ansatz and found that the current is insensitive to the presence of the impurity. From the structure of the Bethe ansatz equations we conjecture that this result holds for any integrable quantum impurity model with an electronic dispersion $\epsilon(k)$ that is an even function of $k$.

²J. acknowledges financial support from the Swedish Research Council through grant 2005-3942.

1:51PM V43.00014 Energy Spectra and Oscillatory Magnetization of Two-Electron Self-Assembled InGaAs/GaAs Ring-like Nanostructures,¹ V.M. FOMIN, V.N. GLADILIN, J.T. DEVREESE, TFVS, Universiteit Antwerpen, Belgium, N.A.J.M. KLEEMANS, H.C.M. VAN GENUCHTEN, P.M. KOENRAAD, PSN, COBRA, TU Eindhoven, The Netherlands — We have analyzed the effect of the Coulomb interaction on the energy spectrum and the magnetization of two electrons in a strained In$_x$Ga$_{1−x}$As/GaAs ring-like nanostructure with realistic parameters inferred from our X-STM data. With increasing magnetic field, the lowest spin-singlet and spin-triplet states sequentially replace each other as the ground state. This is reminiscent of the Aharonov-Bohm effect for the ring-like structures. The exchange interaction leads to a more complicated oscillatory structure of the magnetic moment of the two electrons as a function of the magnetic field as compared to the magnetization pattern for a single-electron ring-like nanostructure. We discuss the relevance of the two-electron systems for the interpretation of the Aharonov-Bohm oscillations in the persistent current observed in low temperature magnetization measurements on self-assembled In$_x$Ga$_{1−x}$As/GaAs ring-like nanostructures.

¹The work has been supported by IUAP, FWO-V project G.0435.03, the WOG WO.035.04N (Belgium) and the EC SANDIE Network of Excellence.
2:03PM V43.00015 Electric-field lithography of LaAlO$_3$/SrTiO$_3$ quasi-two-dimensional electron gas$^1$. CHENG CEN, JEREMY LEVY, STEFAN THIEL, JOCHEN MANNHART — Recent reports$^2,3$ have indicated that the existence of polar discontinuities at the interface between LaAlO$_3$ and SrTiO$_3$ is unstable to the formation of a quasi-two-dimensional electron gas. Below a critical thickness, electrons can still accumulate at the interface under the influence of an applied electric field. We use a biased conducting atomic force microscope (AFM) probe to create conducting nanowires at the LaAlO$_3$/SrTiO$_3$ interface without physical alteration of the interface. The conducting regions written by AFM probe can be written and erased repeatedly. This form of quasi-two-dimensional lithography demonstrates the utility of the LaAlO$_3$/SrTiO$_3$ interface as a rewritable medium, with the potential for creating passive as well as active circuits such as field-effect transistors. (2 A. Ohtomo and H. Y. Hwang, Nature 427, 423 (2004). 3 S. Thiel, G. Hammerl, A. Schmehl, C. W. Schneider, and J. Mannhart, Science 313, 1942 (2006).)

Thursday, March 8, 2007 2:30PM - 5:30PM Session W1 DCMP: Quantum Coherence in Superconducting Devices Colorado Convention Center Four Seasons 2-3

2:30PM W1.00001 Flux Qubits: Coupling and Decoherence$^1$, JOHN CLARKE, University of California, Berkeley — The principles of the three-junction flux qubit are briefly reviewed. We investigated two such qubits coupled together via their mutual inductance and via the dc SQUID (Superconducting Quantum Interference Device) that reads out their magnetic flux states. On-chip flux lines enabled us to bias the two qubits individually. Microwave spectroscopy revealed that the energy splittings of the symmetric and antisymmetric states of the two qubits at their respective degeneracy points were remarkably close, 8.872 GHz and 8.990 GHz. At the double degeneracy point, the energy difference between the first and second excited states of the coupled qubits was enhanced by level repulsion as predicted. We performed time domain measurements on the individual qubits and on excited states of the coupled qubits, including Rabi oscillations, flux echoes, Ramsey fringes and measurements of the relaxation time, and also determined the line widths of the individual peaks. These measurements enable us to compare the relaxation and decoherence rates of the individual and coupled qubits. For example, at the double degeneracy point of the coupled qubits, the decoherence rate determined by flux echoes is equal to the sum of the rates in the separate qubits. Sources of decoherence are discussed, and estimates given of the various known contributions including those of the biasing and measurement circuitry. This work was performed in collaboration with T. Hime, B.L.T. Plourde, P.A. Reichhardt, T.L. Robertson, A.V. Ustinov and C.-E. Wu.

3:06PM W1.00002 Mach-Zehnder Interferometry and Microwave-Induced Cooling in Persistent-CURRENT Qubits, WILLIAM OLIVER, MIT Lincoln Laboratory — Superconducting persistent-current qubits are quantum-coherent artificial atoms with multiple energy levels. In the presence of large-amplitude harmonic excitation, the qubit state can be driven through one or more of the energy-level avoided crossings. The resulting Landau-Zener transitions mediate a rich array of quantum-coherent phenomena as a function of the driving amplitude and frequency. In this talk, we present three such demonstrations of quantum coherence in a strongly-driven niobium persistent-current qubit. The first is Mach-Zehnder-type interferometry [1], for which we observe quantum interference fringes for 1-50 photon transitions. The second is a new operating regime exhibiting coherent quasi-classical dynamics [2], for which theMZ quantum interference persists even for driving frequencies smaller than the resonance linewidth. The third is microwave-induced cooling [3], for which we achieve effective qubit temperatures ~3 mK, a factor 100-1000x lower than the dilution refrigerator ambient temperature. These experiments exhibit a remarkable agreement with theory, and are extensible to other solid-state qubit modalities. In addition to our interest in these techniques for fundamental studies of quantum coherence in strongly-driven solid-state systems, we anticipate they will find application to nonadiabatic qubit control and state-preparation methods for quantum information science and technology. [1] W.D. Oliver, Y. Yu, J.C. Lee, et al., Science 310, 1653 (2005). [2] D.M. Berns, W.D. Oliver, S.O. Valenzuela et al., PRL 97, 150502 (2006). [3] S.O. Valenzuela, W.D. Oliver, D.M. Berns, et al., Science (2006).

3:42PM W1.00003 Vacuum Rabi oscillations observed in a flux qubit LC-oscillator system$^1$, KOUICHI SEMBA, NTT Basic Research Laboratories, NTT Corporation — Superconducting circuit containing Josephson junctions is one of the promising candidates as a quantum bit (qubit) which is a essential ingredient for quantum computation [1]. A three-junction flux qubit [2] is one of such candidates. On the basis of fundamental qubit operations [3,4], the cavity QED like experiments are possible on a superconducting chip by replacing an atom with a flux qubit, and a high-Q cavity with a superconducting LC-circuit. By measuring qubit state just after the resonant interaction with the LC harmonic oscillator, we have succeeded in time domain experiment of vacuum Rabi oscillations, exchange of a single energy quantum, in a superconducting flux qubit LC harmonic oscillator system [5]. The observed vacuum Rabi frequency 140 MHz is roughly 2800 times larger than that of Rydberg atom coupled to a single photon in a high-Q cavity [6]. This is a direct evidence that strong coupling condition can be rather easily established in the case of macroscopic superconducting quantum oscillator system. This work was supported by JSPS KAKENHI (18201018), MEXT KAKENHI (18001002) and JST-CREST.

4:18PM W1.00004 Controllable coupling of superconducting flux qubits$^1$. EVGENI IL’ICHDEV, Institute for Physical High Technology, P.O. Box 100239, D-07702 — As a first step, by making use of conventional niobium technology, we have implemented controllable flux coupling between two qubit prototypes (in our case single junction interferometers) by using a third one as the coupler. The fabricated qubit prototypes operate in the hysteretic mode, where the screening parameter >1, which provides double degenerate state for an external flux equal to half a flux quantum. The coupler parameters were chosen so that it operates in the non-hysteretic mode with a screening parameter of 0.9. The coupling amplitude is proportional to the derivative of the coupler’s current-flux relation. By changing the coupler’s magnetic flux, we have shown ferromagnetic as well as anti-ferromagnetic coupling between the interferometers. In particular, we have demonstrated that the coupling could also be switched off. As the next step of our investigation we implemented similar ideas in to our Al shadow-evaporation technology. Recently, we have also demonstrated a tuneable coupling between three junctions persistent current qubits in the quantum regime. A possible combination of Al and Nb technologies is discussed.

1This work was partly supported by JSPS KAKENHI (18201018), MEXT KAKENHI (18001002) and JST-CREST.

1support of EU projects EuroSQIP and RSFQubit is gratefully acknowledged.
This presentation will discuss the effects of spin-orbital coupling on magnetoresistance tuning through exciton dissociation and exciton-charge reaction in organic semiconductors. Based on this intermolecular spin-orbital interaction, metal electrode-dependent spin-orbital coupling and magnetoresistance have been demonstrated. Interaction modifies the singlet/triplet exciton ratio, changing further charge injection when the space charge carriers from exciton dissociation are considered. Spin-orbit coupling also provides a versatile method for ultrafast luminescence based molecular thermometry. As a first approximation we model the environment by the stray capacitance and stray inductance of the junction electrodes. The total system consisting of the junction and stray elements has two degrees of freedom resulting in two characteristic resonance frequencies. Both frequencies have to be considered to describe the quantum mechanical behavior of the Josephson circuit. 

References:

Thursday, March 8, 2007 2:30PM - 5:30PM –
Session W3 DCMP: Magnetotransport in Organic Conductors and Semiconductors Colorado Convention Center Korbol 2A-3A

2:30PM W3.00001 Spins and Organic Materials: The Spin-dependent OLED, KONRAD BUSSMANN, Naval Research Laboratory — No abstract available.

3:06PM W3.00002 Spin correlations in organic semiconductors, JOHN LUPTON, Department of Physics, University of Utah — Organic semiconductors differ from their inorganic counterparts by large exchange interactions and weak spin orbit coupling. As a result, parallel and anti-parallel spin configurations are highly non-degenerate and spectroscopically well-defined. Whereas singlet excitons are highly emissive, triplet excitons generally decay non-radiatively. Addition of heavy metal elements to the polymer backbone induces localized spin-orbit coupling, which can activate radiative triplet decay through phosphorescence. By tuning the concentration of these triplet acceptors to match the diffusion length of the triplets (which exceeds that of the singlets), triplets can be harvested radiatively without significantly affecting the actual triplet formation pathway through intersystem crossing of the singlet. Using this technique we can study the interconversion between spin states of exciton precursors (charge carrier pairs) as a function of time, temperature, and electric and magnetic fields. We find that the probability of a spin change occurring in the exciton precursor state is extremely small, which suggests that the primary recombination pathway in organic light-emitting diodes is governed by spin statistics. Phosphorescence spectroscopy of organic semiconductors has a number of immediate applications. Stimulated emission competes with intersystem crossing required for triplet generation so that a phosphorescent polymer laser acts as a highly non-degenerate all-optical excitonic switch. Singlet-triplet mixing in metallorganics with strong spin-orbit coupling also provides a versatile method for ultrafast luminescence based molecular thermometry.

References:

3:42PM W3.00003 Characterization and Application of Large Magnetoresistance in Organic Semiconductors, MARKUS WÖHLGENANNT, University of Iowa — Recent years have seen a surge in interest in magnetoresistive and spintronic properties of organic semiconductors, whereas this field was previously almost exclusively concerned with their electrooptical properties. We report on the extensive experimental characterization of a recently discovered large and intriguing magnetoresistive effect in organic light-emitting diodes that reaches up to 10% at room temperature for magnetic fields, B = 10mT. This magnetoresistive effect is therefore amongst the largest of any bulk material. The study includes a range of materials that show greatly different chemical structure, mobility, hyperfine and spin-orbit coupling strength. We show that the applied magnetic field affects the carrier transport inside the bulk semiconductor. By demonstrating that the effect is critically altered by the presence of strong spin-orbit coupling and that it does not occur in fullerene devices, we prove that the transport in organics sensitively depends on spin-dynamics induced by hyperfine interaction with the hydrogen protons. We discuss a possible relation between organic magnetoresistance and other magnetic field effects in organics that were known long before its discovery. As a possible mechanism we describe how Pauli's principle restricts carrier hopping between singly occupied sites near the Fermi level. However, spin-mixing by the hyperfine interaction may partially lift this restriction. Since the devices we describe can be manufactured cheaply they hold promise for applications where large numbers of magnetoresistive devices are needed, such as magnetic random-access-memory (MRAM), and applications related to organic light-emitting diodes such as touch screens where the position of a magnetic stylus is detected (patent pending). We will show a video of a simple demonstrator device.

4:18PM W3.00004 Spin-Orbital Coupling and Magnetoresistance Tuning in Organic Semiconductors, BIN HU, University of Tennessee — Magnetoresistance can be readily obtained from non magnetic organic semiconductors in light-emitting diodes. Tuning this novel magnetoresistance is an important issue in using an external magnetic field to control optoelectronic response in organic semiconductors. The experimental results indicate that uniform mixing of strong spin-orbital-coupling fac-tris(2-phenylpyridinate) iridium [Ir(ppy)$_3$] molecules and weak-spin-orbital-coupling poly(N-vinyl carbazole) (PVK) leads to a concentration-dependent magnetoresistance. There are three possible processes, namely intermolecular spin-orbital interaction, energy transfer, and charge transport, that can contribute to the concentration-dependent magnetoresistance. The magnetic field-dependent electroluminescence shows that an intermolecular spin-orbital interaction is formed in the PVK-Ir(ppy)$_3$ mixture. This intermolecular spin-orbital interaction modifies the singlet/triplet exciton ratio, changing further charge injection when the space charge carriers from exciton dissociation are considered. Based on this intermolecular spin-orbital interaction effects, metal electrode-dependent spin-orbital coupling and magnetoresistance have been demonstrated. This presentation will discuss the effects of spin-orbital coupling on magnetoresistance tuning through exciton dissociation and exciton-charge reaction in organic light-emitting diodes through controlling energy transfer and bipolar injection.

This work was supported by NSF Grant No. ECS 04-23911,
4:54PM W3.00005 Low Field, Large Magnetoresistance in Nonmagnetic Organic Semiconductors\textsuperscript{1} JEREMY D. BERGESON\textsuperscript{2}, Dept. of Physics, The Ohio State University, Columbus, OH 43210-1117 — Transport in various thin-film organic semiconductors has been shown to have an anomalously high sensitivity to low magnetic fields at room temperature (RT). Early experiments on polydiacetylene single crystals and poly(phenylenevinylene) revealed increases in photoconductivity of a few percent at RT\textsuperscript{3}. Further magnetotransport studies showed larger effects in \pi-conjugated backbone polymers and small molecules\textsuperscript{4}. We report magnetoresistance (MR) for semiconducting oligomer and nonconjugated polymer materials in addition to small molecule and conjugated backbone polymer materials. For example, films of the light emitters poly(N-vinylcarbazole) and Alq\textsubscript{3} each have an MR response greater than 5\% at an unusually low magnetic field of 100 Oe (\mu_0 H \sim 0.0006 meV) at an unusually high temperature of 300 K (k_BT \sim 26 meV). Increasing the spin-orbit coupling in Alq\textsubscript{3} films by doping with the phosphorescent sensitizers Ir(ppy)\textsubscript{3} or PtOEP strongly suppresses the MR signal. MR in thin films of the oligomer \alpha-sisithiophene can be negative, similar to the behavior of other organic semiconductors, or positive depending on the temperature, layer thickness, or applied voltage. We have developed a model, termed Magnetoresistance by the Interconversion of Singlets and Triplets (MIST), accounting for this anomalous MR\textsuperscript{5}. At zero field, the singlet and triplet e-h pair states are degenerate and the states can readily interconvert due to hyperfine interaction. Finite magnetic fields lift triplet degeneracy which affects the hyperfine interconversion of e-h pairs between singlet and triplet states. By changing the carrier recombination the MIST mechanism gives rise to a space-charge-limited current that depends on magnetic field, producing MR.

\textsuperscript{1}This work supported by AFOSR Grant No. FA9550-06-1-0175 and DOE Grant Nos. DE-FG02-86ER45271 and DE-FG02-01ER45931.

\textsuperscript{2}In collaboration with V.N. Prigodin, D.M. Lincoln and A.J. Epstein.


\textbf{Thursday, March 8, 2007 2:30PM - 5:30PM — Session W7 DCMP: Novel Phenomena in Quantum Fluid He-3 Colorado Convention Center Korbel 4A-4B}

2:30PM W7.00001 Transport in highly spin-polarized normal liquid 3He. PIERRE-ETIENNE WOLF, Institut Néel-CNRS, Grenoble — Normal liquid Helium 3 is an ideal system to study the role of correlations in fermions physics. It is characterized by strong interactions between particles, the range of which is comparable to the inter-atomic distance. As such, it represents an intermediate case of complexity, halfway between the electronic systems and the ultra-cold Fermi gases. In particular, transport in degenerate Helium 3 involves not only s-wave scattering, but also partial waves with non-zero orbital angular momentum. Studying the polarization dependence of transport allows to directly probe this fact. We will report on transport experiments in a highly spin-polarized, degenerate, liquid 3He, obtained by melting spin polarized solid 3He and rapidly cooling the resulting liquid down to about 60 mK. While the polarization dependence of viscosity is unexpectedly close to that predicted for a free fermion gas, the thermal conductivity increases much less with polarization than expected in that case. We will discuss the possible reasons for this difference.

3:06PM W7.00002 Magnetic Relaxation and Minority Spin Condensate in Spin-Polarized Superfluid 3He A\textsubscript{1} HARRY KOJIMA, Rutgers University — The magnetic relaxation phenomena in superfluid 3He A\textsubscript{1} phase are studied using a magnetic fountain pressure detector in which a large reservoir is connected to a small sensor chamber through two superleak channels of height 18 \mu m. Superflow in simultaneous mass/spin current is driven by an externally applied magnetic field. Measurements of the relaxation of the induced fountain pressure are carried out under a variety of conditions including pressure(3 - 29 bar), temperature, static field(up to 8 T) and 4\textsuperscript{He}(5 monolayers) coverage. The relaxation of the fountain pressure arises from the time dependent spin polarization in the sensor chamber. The observed relaxation time \tau varies from 80 s near the upper transition temperature, T_c1, to less than 0.1 s near the lower transition temperature, T_c2. The measured relaxation rate increases starting near the middle of A\textsubscript{1} phase and more rapidly as T_c2 is approached. The 4\textsuperscript{He} coverage is observed not to affect the measured spin relaxation rate and this indicates that the relaxation is a bulk liquid effect. The rapid increase in relaxation rate is interpreted in terms of the Leggett-Takagi\textsuperscript{1} mechanism of intrinsic spin relaxation arising from a small but increasing presence of minority spin pair condensate\textsuperscript{2} with magnetic moment aligned in the opposite direction to the applied field) in A\textsubscript{1} phase as T_c2 is approached. It is concluded that the conventional view of the superfluid A\textsubscript{1} phase being composed of condensate pairs with magnetic moment aligned strictly along the applied field is inadequate.


In collaboration with A. Yamaguchi, S. Kobayashi and H. Ishimoto. Supported in part by NSF, MEXT and JSPS.

3:42PM W7.00003 Specific Heat of Superfluid 3He and Andreev Bound States, WILLIAM HALPERIN, Northwestern University — The specific heat at the normal to superfluid transition gives a clear thermodynamic signature for onset of the superfluid state marked by a discontinuity which has been accurately determined by Greywall\textsuperscript{1}. We have measured the effect of a silver surface on the specific heat at this transition and we have found a temperature dependent suppression of the specific heat in the superfluid state which we have studied as a function of temperature and pressure\textsuperscript{2}. This result can be understood in terms of the contribution to the Free energy from surface Andreev bound states which have a range of half of a superfluid coherence length. For the case of very large surface-to-volume ratio, as can be achieved with high porosity silica aerogel, the superfluid transition is suppressed. We have measured the specific heat anomaly at the transition temperature for this case\textsuperscript{3} and interpret our measurements in terms of scattering theory. At the lowest temperatures a band of Andreev surface bound states dominate the specific heat of the superfluid 3He/aerogel system. This work was performed in collaboration with H. Choi, J.P. Davis, and J. Pollanen at Northwestern University, supported by the NSF grant DMR-0244099. [1] D.S. Greywall, Phys. Rev. B, 33, 7520, (1986). [2] H. Choi, J.P. Davis, J. Pollanen, and W.P. Halperin, Phys. Rev. Lett. 96, 125301 (2006). [3] H. Choi, K. Yawata, T.M. Haard, J.P. Davis, G. Gervais, N. Mulders, P. Sharma, J.A. Sauls, and W.P. Halperin, Phys. Rev. Lett. 93, 145301 (2004).

4:18PM W7.00004 Surface Andreev Bound States of 3He-B by Transverse Acoustic Impedance Measurements, YUICHI OKUDA, Tokyo Institute of Technology — Complex transverse acoustic impedance of the superfluid 3He was measured at the frequencies of 10 to 80 MHz from 6 up to 25 bar by a CW bridge method. The observed temperature dependence of it was well explained by the quasi-classical theory with random S-matrix model for a diffusive surface. The impedance was influenced by pair breaking and by quasi-particle density of states at the surface, which was drastically modified from the bulk one by the formation of surface Andreev bound states. In B phase, an additional gap in SDOS opened between the upper energy edge \Delta' of the surface Andreev bound states band and the bulk energy gap \Delta. Temperature dependence of \Delta' was measured and was about 30\% smaller than theoretical values. In A phase, flat and gapless SDOS was confirmed experimentally for the first time. It is demonstrated that the present spectroscopic method is a good tool to investigate the surface microscopic state, which has not been possible for the charge neutral p-wave superfluid.
Phase separation and electron pairing in repulsive Hubbard clusters illustrates how these features are scaled with cluster size. The phase diagram for 2 x 4-site clusters illustrates how these features are scaled with cluster size. The phase diagram of half filling strongly suggests existence of subsequent transitions from electron pairing into unsaturated ferromagnetic and saturated ferromagnetic Mott-Hubbard like insulators driven by electron repulsion. Rigorous criteria for occurrence of corresponding quantum critical points and crossover temperatures are formulated. The phase diagram for 2 x 4-site clusters illustrates how these features are scaled with cluster size. The phase separation and electron pairing monitored by magnetic field and electron doping surprisingly resemble phase diagrams in family of doped high Tc cuprates. [1] Phys. Rev. B 74, 024511, [2] (2006) cond-mat/0608579 (2006)
3:42PM W11.00007 Ferromagnetism in the one-band Hubbard Model on a triangular lattice1. SHI-QUAN SU, Department of Physics, The Chinese University of Hong Kong, ZHONG-BING HUANG, Department of Physics, Hubei University, Hubei, China, RUI FAN, HAI-QING LIN, Department of Physics, The Chinese University of Hong Kong — We investigated numerically the existence of ferromagnetic phase in the one-band Hubbard model on a triangular lattice. By studying the spin susceptibility, we found the model exhibits ferromagnetic properties when the density of electrons is low. Auxiliary Field Quantum Monte Carlo (AFQMC) and Constrained Path Monte Carlo (CPMC) data are used to present the system behaviors including spin susceptibility, pair correlation, when the parameters of the model change. We found that these behaviors are related to the ferromagnetism of the model. These results can be viewed as evidences to support a route to metallic ferromagnetism in the one-band Hubbard models.

1Work supported partially by HKSAR RGC 401806.

3:54PM W11.00008 Novel Electronic Properties of the Hubbard Model on a Frustrated Triangular Lattice1.BUMSOO KYUNG, University of Sherbrooke — We study novel electronic properties of the Hubbard model on a triangular lattice using the cellular dynamical mean-field theory. The interplay of strong geometric frustration and electron correlations causes a Mott transition at the Hubbard interaction $U/t = 10.5$ and an unusual suppression of low energy spin excitations. Doping of a triangular Mott insulator leads to a quasiparticle peak (no pseudogap) at the Fermi surface and to an unexpected increase of low energy spin excitations, in stark contrast to the unfrustrated square lattice case. The present results give much insight into strongly frustrated electronic systems. A few predictions are made. cond-mat/0608202

1NSERC (Canada), FQRNT (Qu´ebec), CFI (Canada), and CIAR

4:06PM W11.00009 Luttinger Liquid Kink. TRINANJAN DATTA, ERICA W. CARLSON, JIANGPING HU, Purdue University — We consider a spin rotation invariant Luttinger Liquid at finite temperature and show the existence of a kink in the effective dispersion, as determined by the frequency-dependent peak in the momentum distribution curve (MDC). The MDC is defined by considering the single hole spectral function $A^< (\vec{k}, \omega)$ as a function of $\vec{k}$ at a fixed frequency $\omega$. When the charge velocity is greater than the spin velocity, $v_c > v_s$, the high frequency dispersion is linear in $\vec{k}$ and follows $v_c$, while the low frequency dispersion (which is also linear in $\vec{k}$) follows some average of the two velocities. The energy scale of the crossover between the two velocities defines a kink, $E_{\text{kink}}$. Since the Luttinger Liquid is quantum critical, $E_{\text{kink}}$ scales with the temperature. The kink energy is also affected by the interaction strength, and the strength of the kink is controlled by the ratio of the spin and charge velocities.

AUXILIARY FIELDS FRAGMENTS FOR METALS AND ALLOYS

4:18PM W11.00010 Heisenberg spin chains with four-spin couplings1. ALEXIOS KLIRONOMOS, JULIA MEYER, Department of Physics, The Ohio State University, 191 W Woodruff Ave, Columbus OH 43210, USA, TOSHIYA HIKIHARA, Department of Physics, Hokkaido University, Sapporo 060-0810, Japan, Konstantin Matveev, Materials Science Division, Argonne National Laboratory, USA — We obtain and analyze the phase diagram of the zigzag Heisenberg spin chain including four-spin interactions arising from ring exchange processes. We perform exact diagonalization of chains up to 24 sites. In addition to the expected ferromagnetic, antiferromagnetic and dimer phases, the phase diagram contains a region of partial spin polarization as well as a region occupied by novel phase(s).

1This work was supported by the U. S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357. Part of the calculations were performed at the Ohio Supercomputer Center thanks to a grant of computing time.

4:30PM W11.00011 Phase diagram of the one dimensional Hubbard-Holstein Model at 1/2 and 1/4 filling1. RAHUL HARDIKAR, TORSTEN CLAY, Mississippi State University — We present a detailed study of the phase diagram of the Hubbard-Holstein model at 1/2 filling and 1/4 filling, including finite-frequency quantum phonons within the numerically exact Stochastic Series Expansion quantum Monte Carlo method. In one dimension at 1/2 filling, the electron-phonon (e-ph) coupling gives a Peierls charge density wave, while Hubbard onsite $U$ promotes antiferromagnetic correlations and a Mott insulating state. Our previous study revealed a third Intermediate phase when the electron-electron and e-ph interaction are closely balanced. We show here from direct calculations of charge and spin susceptibilities that (i) as the e-ph coupling strength is increased first a spin gap transition and then the Peierls transition occurs, (ii) transitions between Mott/Intermediate and Intermediate/Peierls states are of the Kosterlitz-Thouless type, (iii) for large $U$, the two transitions merge into a single first order transition. Our data is consistent with a renormalization of the Luttinger Liquid exponent $K_\rho$, which gives a slightly larger intermediate region as determined from susceptibilities than in previous calculations of $K_\rho$. At 1/4 filling we find a very similar phase diagram.

1Supported by the American Chemical Society (Petroleum Research Fund) and DOE

4:42PM W11.00012 Deformation of SU(4) singlet spin-orbital state due to Hund’s rule coupling. HIROAKI ONISHI, TAKASHI HOTTA, Advanced Science Research Center, Japan Atomic Energy Agency — It has been widely recognized that the interplay of spin and orbital degrees of freedom plays a crucial role in the emergence of novel magnetism in strongly correlated systems. In this context, a one-dimensional spin-orbital model with the highest SU(4) symmetry has been one of the subjects of much interest from a theoretical viewpoint, and the critical behavior of the SU(4) singlet ground state has been clarified. However, in a more realistic situation, the Hund’s rule coupling should break the SU(4) symmetry. In the present work, by exploiting a density-matrix renormalization group method, we investigate a one-dimensional spin-orbital model in which the SU(4) symmetry is broken down to SU(2)$_{\text{spin}} \times U(1)_{\text{orbital}}$ due to the Hund’s rule coupling ($J$). At $J = 0$, spin and orbital correlations coincide with each other with a peak at $q = \pi/2$, indicating the SU(4) singlet state with a four-site periodicity. On the other hand, with increasing $J$, the peak position of orbital correlation changes to $q = \pi$, while that of spin correlation remains at $q = \pi/2$. We will discuss in detail how the SU(4) singlet state is deformed by the Hund’s rule coupling.

Thursday, March 8, 2007 2:30PM - 5:30PM – Session W23 DCMP: Metals: Alloys and Compounds Colorado Convention Center 110
2:30PM W23.00001 Anomalous electronic correlations in ground state momentum density of Al$_{77}$Li$_{3}$, B. BARBIELLINI, Northeastern U., J. KWIAKTOWSKA, Polish Academy of Sciences (Poland), S. KAPRZYK, Northeastern U. and AGH (Poland), A. BANSIL, Northeastern U., H. KAWATA, N. SHIOTANI, Photon Factory (Japan) — We report high resolution Compton scattering measurements on an Al$_{77}$Li$_{3}$ disordered alloy single crystal for momentum transfer along the [100], [110] and [111] symmetry directions [1]. The results are interpreted via corresponding KKR-CPA (Korringa-Kohn-Rostoker coherent potential approximation) first principles computations. By comparing spectra for Al$_{77}$Li$_{3}$ and Al, we show that the momentum density in the alloy differs significantly from the predictions of the conventional Fermi liquid picture and that the ground state of Al is modified anomalously by the addition of Li. Work supported in part by the USDOE.


2:42PM W23.00002 Pseudo-gap observed at martensite transition in Ni$_{52}$MnGa single crystal, C.P. OPEIL, Boston College, J.C. LASHLEY, R.K. SCHULZE, B. MIHAILA, W.L. HULTS, J.L. SMITH, Los Alamos National Laboratory, P.S. RISEBOROUGH, Temple University, L. MANOSA, A. PLANES, Universitat de Barcelona — Specific heat and coefficient of linear thermal expansion coefficient measurements show that the ferromagnetic shape-memory alloy Ni$_{52}$MnGa single crystal exhibits a pre-martensitic transition (PMT) at T = 214 K and a martensitic transition (MT) at 196 K. Lee et al. predicts that magnetically-tuned Fermi-surface nesting at q = (2π/3a) (1,1,0) is responsible for phonon softening at the PMT. On the basis of temperature dependence of the PMT and photoemission measurements, we show that a pseudo-gap opens at 0.3 eV below the Fermi energy at the martensitic transition (MT) thus providing further evidence that the Fermi surface is nested at the MT and is only partially nested at the PMT.

3:06PM W23.00004 Electronic structure theory of the structural transformation of shape memory NiTi, NICHOLAS HATCHER, OLEG KONTSEVOI, ARTHUR FREEMAN, Northwestern University — The unique property of displacive phase transformations has created much interest in the study of martensitic materials. Among them, NiTi finds a wide range of applications due to its shape memory behavior, however, the detailed mechanism of its structural evolution during the martensitic transformation is not fully understood. We have investigated the transformation paths between the B2, R, B19, and B19' phases using the highly-precise FLAPW method to identify the governing processes of the transformation through calculations of the total energy, electronic structure, elastic moduli, and shear energetics. For example, we show the role of topological shifts of the Fermi surface and band structure evolution with the changing monoclinic angle of the B19' and R phases. In addition, the magnetism and magnetic susceptibility of the phases are investigated using both fixed spin moment and Stoner enhancement calculations. To date, we find the B2, B19, and B19' phases to be Stoner enhanced paramagnets.

3:18PM W23.00005 Possible metastable rhombohedral states of the bcc transition metals, MICHAEL MEHL, DANIEL FINKENSTADT, Center for Computational Materials Science, Naval Research Laboratory, Washington DC — The energy E(c/a) for a bcc element strained along its [001] axis (the Bain path) has a minimum at c/a = 1, a maximum at c/a = √2, and an elastically unstable local minimum at c/a = √3. A rhombohedral strain is an alternative method of connecting the bcc and fcc structures. The primitive lattice keeps R3m symmetry, with the angle α changing from 109.4° (bcc), to 90° (simple cubic), to 60° (fcc). We studied this path for the non-magnetic bcc transition metals (V, Nb, Mo, Ta, and W) using both a full-potential LAPW and PAW VASP. Except for Ta, the energy E(α) has a local maximum at α = 60°, with local minima near 55° and 70° the later having lower energy. We studied the elastic stability of the 70° minimum structure. Only W is elastically stable in this structure, with the smallest eigenvalue of the elastic tensor at 4 GPa, while the other three elements are unstable. We discuss the possibility that Tungsten is actually metastable in this structure. We also consider the possible epitaxial growth of this structure.

3:30PM W23.00006 The pressure-induced bcc-hcp structural transformation in iron, BABAK SADIGH, MICHEAL SURH, Lawrence Livermore National Laboratory — We study within the framework of the spin density-functional theory the microscopic mechanism of the bcc-to-hcp martensitic transformation in iron from first principles. We investigate the correlation of the pressure-induced structural instability of the bcc phase with the disappearance of ferromagnetism in this system. We show that our calculations can shed new light on recent novel shock experiments in single-crystalline iron.

3:42PM W23.00007 Prediction of a metastable cubic phase for the transition metals with hcp ground state. ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico, AARON AGUAYO, GABRIEL MURRIETA, Facultad de Matematicas, UADY, Mexico — The discovery of a metastable phase for a given material is interesting because it corresponds to a new bonding and new properties are expected. The calculation of the total-energy along the Bain path is frequently used as a method to find tetragonal metastable states. However, a local minimum in the tetragonal distortion is not a definitive proof of a metastable state, and the elastic stability needs to be evaluated. In a previous work, using the elastic stability criteria for a cubic structure, we have shown that the transition metals with hcp ground state; Ti, Zr, and Hf have a fcc metastable phase [Aguayo, G. Murrieta, and R. de Coss, Phys. Rev. B 65, 092106 (2002)]. That result is interesting since the fcc crystal structure does not appear in the current pressure-temperature phase diagram of these metals, and support the experimental observations of fcc Ti and Zr in thin films. In the present work, we extend the elastic stability study of the fcc structure to the non-magnetic transition metals with hcp ground state; Sc, Ti, Y, Zr, Tc, Ru, Hf, Re, and Os. We find that all the metals involved in this study have a metastable fcc structure. From these results, substrates on which the fcc structure of these metals could be growth epitaxially are predicted.
3:54PM W23.00008 Anharmonic Phonons in Vanadium Alloys and Compounds. OLIVIER DELAIRE, MAX KRESCH, MATTHEW LUCAS, REBECCA STEVENS, CALTECH, JORGE MUNOZ, UTEP, BRENT FULTZ, CALTECH — Using inelastic neutron scattering, we investigated the temperature-dependence of the phonon density of states (DOS) of pure BCC vanadium and vanadium alloys V-6.25%X, with X a transition metal solute, as well as the A15 compounds V3Si and V3Ge. Phonons in pure vanadium exhibit an anomalously softer thermal expansion with increasing temperature up to 1000°C. The addition of 6.25% impurities in solid solution changes this behavior. Solutes to the right of vanadium in the periodic table induce a reversal to the expected quasiharmonic softening with thermal expansion, solutes to the left increase the stiffening. V3Si and V3Ge also exhibit strong phonon stiffenings up to 500°C. Anharmonic couplings arising from phonon-phonon or electron-phonon interactions are used to explain the departure from the quasiharmonic behavior. Using differential scanning calorimetry, we measured the heat capacity of vanadium and its alloys up to 1400°C, and related it to the temperature-dependent phonon DOS. We compare our findings to theoretical studies of the effect of phonon-phonon and electron-phonon couplings on the heat capacity.

4:06PM W23.00009 Ab-initio calculations of phonon properties for the Nb-Mo alloy using the virtual crystal approximation. O. DE LA PEÑA-SEAMAN, R. DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico, R. HEID, K.-P. BOHNEN, Institut fuer Festkoerperfysik, Forschungszentrum Karlsruhe, Germany — We have studied the structural, electronic, and lattice dynamic properties of the Nb_{1-x}Mo_{x} alloy within the framework of the density functional perturbation theory, using the mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloy. The calculations were performed for both LDA and GGA xc-functional approximations. The structural parameters were optimized via the total-energy method for the whole range of Mo-concentration (0 ≤ x ≤ 1). The electronic properties were analyzed in terms of the electronic topological transitions (ETT) in the Fermi surface. The calculated phonon dispersion curves for the different Mo-concentrations are in very good agreement with experimental data reported in the literature. We find that LDA results are in general higher in frequency than GGA. The evolution of the Kohn anomaly in the I'H direction observed experimentally in the Nb-Mo alloy is well reproduced by the VCA calculations. Thus, we have shown that the virtual crystal approximation as implemented in the present work is useful for the study of random intermetallic alloys where the alloying elements are adjacent in the periodic table. This research was supported by CONACYT, Mexico under Grant No. 43830-F.

4:18PM W23.00010 Electronic Grüneisen Parameter in the Non-equilibrium Regime. JINCHENG WANG, CHUNLEI GUO, University of Rochester — The Grüneisen parameter is a fundamental parameter characterizing the relationship between thermal expansion and specific heat of a solid. Conventionally, electronic Grüneisen parameter γ_e is measured in a solid by minimizing the lattice contribution to thermal expansion at low temperatures, and the value of γ_e is believed to be a constant. In this report, we perform pump-probe experiments using surface plasmon as the probe technique to resolve the dynamics of acoustic phonons that are impulsively excited in Ag film using fs laser pulses. Our study shows that the conventional value of electronic Grüneisen parameter is not necessarily valid in thermal non-equilibrium distribution immediately following ultrafast pulse excitation. A revised γ_e is proposed here to precisely take into account the role of electron pressure in driving acoustic phonons in solids.

4:30PM W23.00011 A new intermetallic prototype? Verifying new structure predictions in CdPt and PtPd by first-principles. GUS HART, Brigham Young University — A recent data-mining approach to predicting the structure of intermetallic compounds has suggested that the CdPt and PtPd systems harbor a new crystal structure. Unlike other such predictions, this one is unique. The structure, never seen in any other fcc-based intermetallic, contains only four atoms per unit cell. Furthermore, this structure is the only one of this small size, except L12, that cannot be characterized as a sequential stacking of planes containing only A or B atoms. The stability of such a structure is tested using an exhaustive search of a unit cell-structures (L10, L11, DO22, etc) or as “Long Period Superstructures” (LPS) having huge cells. Examples of the latter are the 1D polytypes of SiC.

4:42PM W23.00012 Novel ground states in mixed bcc/fcc, high-/low-spin Fe-(Ni,Pd,Pt) from first-principles. SERGEY V. BARABASH, ROMAN V. CHEPULSKII, VOLKER BLUM, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO 80401 — Among the observed ordered phases of Fe-X (X=Ni,Pd,Pt), some structures are curiously absent: L10 FePd and FeNi do not; L12 FePt and FePd exist, but the stability of L10 FeNi is debated. Furthermore, the recently measured short range order (SRO) in Fe-rich Fe-Ni is at odds with L12-type SRO. Theory has been hindered by the appearance of geometric (bcc/fcc) and magnetic (high-spin [HS]/low-spin [LS]) bi-stabilities. We address such bi-stabilities by performing first-principles mixed-basis cluster expansion with added geometric and magnetic filters, separating structures according to HS/LS and “degree” of fcc-ness and bcc-ness. We performed separate fcc HS and (for FePd) bcc HS cluster expansions. We predict that at low temperatures: (i) New ordered structures exist, including fcc Pt3Ti-type FeX4 and the (100) superlattices Fe2Pd and Fe2Pt; (ii) All fcc FeX compounds are unstable w.r.t. bcc Fe + L10 FeX (iii) Fcc FePd is unstable w.r.t. bcc Fe + (100) Fe2Pd superlattice, while L10 FeNi is, in fact, stable w.r.t. bcc Fe + L12 FeNi. At high T, (iv) The SRO in Fe-rich Fe-Ni is governed by (100) superlattice ordering.

-supported by NSF DMR-0650406. 1

4:54PM W23.00013 Are the superstructures seen in the Cu-Pd phase-diagram ground states? First-principles predicted structures. STEFAN MÜLLER, STEFAN BÄRTHLEIN, ELKE WINNING, University Erlangen-Nuernberg, Lehrstuhl fuer Festkoerperfysik, Staudstr. 7, D-91058 Erlangen, Germany, GUS HART, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, Colorado 80401 — Ordered phases appear in nature either as ordinary, small-unit cell-structures (L10, L11, DO22, etc) or as “Long Period Superstructures” (LPS) having huge cells. Examples of the latter are the 1D polytypes of SiC or the 1D and 2D LPS’s seen in the phase diagram of Cu-Pd. Finding via first-principles calculations, if such structures correspond to thermodynamic ground states or represent kinetically frozen-in structures has been hindered by the large number of atoms O(10^3) in such LPS’s. We use instead a set of directly-calculated first-principles total energies to construct a Cluster-Expansion Hamiltonian whose ground states can be rapidly surveyed. We predict for Cu-Pd (i) a yet undiscovered Cu7Pd ( =S1) ground state at X(Pd)= 12.5% and the LPS3 structure ( =S2) at 25%. (ii) In the low-temperature regime a single L12 phase cannot be stable, even at the presence of antisites. Instead we find that an S2-phase with an S1-like ordering tendency will form. (iii) 2D-LPS’s are probably kinetically-stabilized structures which transform into the 1D-LPS ground-state structures in thermal equilibrium.
Cincinnati — We present results from resonant Raman spectroscopy, x-ray photoelectron spectroscopy (XPS) and thermoelectric power (TEP) measurements on boron-doped single-wall carbon nanotubes (B-SWNTs). The structure in the optical spectrum of semiconducting nanotubes while not lowering significantly that of the metallic tubes. At room temperature, we have measured the four-probe sheet resistance and its frequency shifts are related to the change in the diameter distribution of the DWNT sample caused by increasing the heat treatment temperatures. The radial breathing mode spectra we find that the smaller diameter tubes disappear before the larger diameter tubes as the sample is heat treated at higher temperatures. By using different laser excitation energies ranging from 1.57eV to 2.41eV, we observe in agreement with prior work that the outer tubes shield the inner tubes and give rise to the B-C band characteristic lineshape. We also find that the G’ feature contains contributions from the inner and outer layers of a DWNT and its frequency shifts are related to the change in the diameter distribution of the DWNT sample caused by increasing the heat treatment temperatures. Finally, we report on the observation of a four fold splitting of the G’ Raman feature and analyze the similarities with recent studies on 2-layer graphene.

Pennsylvania State University — Thin films of carbon nanotubes have been reported to be a replacement for transparent conducting films of Indium-Tin-Oxide (ITO). Nanotube films can be deposited on flexible plastic and are predicted as a new technology for touch screens, solar cells, etc. Here we report results on thin films of boron-doped single-walled carbon nanotubes (B-SWNTs) obtained from Carbolex, Inc. Boron-doping is expected to raise the conductivity of semiconducting nanotubes while not lowering significantly that of the metallic tubes. At room temperature, we have measured the four-probe sheet resistance and the optical transmission in the NIR-UV range to evaluate the performance of these chemically enhanced SWNT films. The structure in the optical spectrum is essentially the same as in pristine tubes, although the positions of optical absorption bands are slightly upshifted (~1522 cm⁻¹) with oxygen plasma treated SWNTs. These results show that oxygen plasma treatment affects the metallic nanotubes in our sample more than semiconducting ones. The Raman spectra of hydrogen treated SWNTs show a much smaller D band peak than the oxygen treated SWNTs. The G bands of the hydrogen treated SWNTs are also up shifted compared to untreated nanotubes.

Deutsche Bahn AG, Hamburg, Germany — The role of short range order in the determination of higher order correlation in solid solutions is essentially the same as in pristine tubes, although the positions of optical absorption bands are slightly upshifted (~1522 cm⁻¹) with oxygen plasma treated SWNTs. These results show that oxygen plasma treatment affects the metallic nanotubes in our sample more than semiconducting ones. The Raman spectra of hydrogen treated SWNTs show a much smaller D band peak than the oxygen treated SWNTs. The G bands of the hydrogen treated SWNTs are also up shifted compared to untreated nanotubes. The surface of the oxygen plasma treated SWNTs was also analyzed by XPS. These results show that the O1s to C1s intensity ratio is considerably higher in oxygen treated SWNTs compared to untreated nanotubes. The TEP measurements confirm that these plasma treatments induce defects as well as add side wall functionalization to the SWNTs.

YINGZHOU DU, ROBERT MCQUEENNEY, MIAOLIANG HUANG, THOMAS LOGRASSO, DEBORAH SCHLAGE, SUNG CHANG, DOUGLAS ROBINSON, DEPARTMENT OF PHYSICS AND ASTRONOMY, IOWA STATE UNIVERSITY, AMES, IA 50011 TEAM — FeₓGaₓ alloys are known for having large magnetostriction (MS) while maintaining good ductility. Further improvement of the MS properties appears to be limited by Ga ordering. As Ga composition is increased, the MS coefficient is observed to peak, and then drop rapidly, when the system crosses over from a solid solution to an ordered alloy. In our experiments, x-ray diffuse scattering was used to study the Ga short-range order (SRO) as a function of composition and heat treatment. The data indicate the development of DO₂-type SRO with increasing Ga composition in the BCC solid solution. For the slow-cooled samples, the correlation length and area of the SRO scattering both increase dramatically beyond the peak in the MS at x = 0.18, indicating that the development of Ga clusters beyond a certain size limits the MS. The trends for the quenched samples are similar, but not as clear as the slow-cooled ones. The results indicate that nanoscale sized Ga clusters act to enhance the magnetoelastic coupling.

Thursday, March 8, 2007 2:30PM - 5:30PM — Session W31 DCMP: Nano-tubes, Wires, and Dots: Optical and Raman Experiments Convention Center 401

2:30PM W31.00001 Raman Spectroscopy of Heat-Treated Boron Doped Double Wall Carbon Nanotubes⁴, F. VILLALPANDO, H.B. SON, G.G. SAMSONIDZE, Massachusetts Institute of Technology, S.G. CHOU, Pfizer Global Research and Development, Y.A. KIM, H. MURAMATSU, T. HAYASHI, M. ENDO, Shinshi University, M. TERRONES, Instituto Potosino de Investigacion Cientifica y Tecnologica, M.S. DRESSELHAUS, Massachusetts Institute of Technology — We performed Raman spectroscopy experiments on undoped and boron-doped double walled graphene nanotubes that exhibit the “coalescence inducing mode” as they are heat treated at temperatures between 1200C and 2000C. From the radial breathing mode spectral data we find that the smaller diameter tubes disappear before the larger diameter tubes as the sample is heat treated at higher temperatures. By using different laser excitation energies ranging from 1.57eV to 2.41eV, we observe in agreement with prior work that the outer tubes shield the inner tubes and give rise to the B-C band characteristic lineshape. We also find that the G’ feature contains contributions from the inner and outer layers of a DWNT and its frequency shifts are related to the change in the diameter distribution of the DWNT sample caused by increasing the heat treatment temperatures. Finally, we report on the observation of a four fold splitting of the G’ Raman feature and analyze the similarities with recent studies on 2-layer graphene.

2:42PM W31.00002 Optical Transmittance and Sheet Resistance of B-doped Single-Walled Carbon Nanotubes, XIAOMING LIU, HUGO ROMERO, HUMBERTO GUTIERREZ, KOFI ADU, PETER EKLUND, Department of Physics, Pennsylvania State University — Thin films of carbon nanotubes have been reported to be a replacement for transparent conducting films of Indium-Tin-Oxide (ITO). Nanotube films can be deposited on flexible plastic and are predicted as a new technology for touch screens, solar cells, etc. Here we report results on thin films of boron-doped single-walled carbon nanotubes (B-SWNTs) obtained from Carbolex, Inc. Boron-doping is expected to raise the conductivity of semiconducting nanotubes while not lowering significantly that of the metallic tubes. At room temperature, we have measured the four-probe sheet resistance and the optical transmission in the NIR-UV range to evaluate the performance of these chemically enhanced SWNT films. The structure in the optical spectrum is essentially the same as in pristine tubes, although the positions of optical absorption bands are slightly upshifted (~50 meV) relative to pristine SWNTs. The B-loading, microstructure, bonding and defects of the B-doped SWNTs were characterized, respectively, by inelastic neutron scattering, transmission electron microscopy, electron energy loss spectroscopy and Raman spectroscopy. Our preliminary results on B-SWNTs show that the visible optical transmittance is higher and the sheet resistance is much lower than that of similar thickness SWNT films.

2:54PM W31.00003 Raman Spectroscopy Studies of Oxygen and Hydrogen RF-Plasma Treated Single Wall Carbon Nanotubes, CHAMINDA JAYASINGHE, DAVID B. MAST, Department of Physics, University of Cincinnati — We present results from resonant Raman spectroscopy, x-ray photoelectron spectroscopy (XPS) and thermoelectric power (TEP) measurements on hydrogen and oxygen plasma treated single-wall carbon nanotubes (SWNTs). For oxygen treated SWNTs, Raman spectroscopy of the BFW band (~1522 cm⁻¹) show a dramatic up shift for both the ~1522 cm⁻¹ band and the ~1578 cm⁻¹ band by nearly 20 cm⁻¹. In addition, there is a considerable change in the appearance of the D’ mode (~1620 cm⁻¹) with oxygen plasma treated SWNTs. These results show that oxygen plasma treatment affects the metallic nanotubes in our sample more than semiconducting ones. The Raman spectra of hydrogen treated SWNTs show a much smaller D band peak than the oxygen treated SWNTs. The G bands of the hydrogen treated SWNTs are also up shifted compared to untreated nanotubes. The surface of the oxygen plasma treated SWNTs was also analyzed by XPS. These results show that the O1s to C1s intensity ratio is considerably higher in oxygen treated SWNTs compared to untreated nanotubes. The TEP measurements confirm that these plasma treatments induce defects as well as add side wall functionalization to the SWNTs.

Finite Size Effect in ZnO Nanowires

3:18PM W31.00005 Finite Size Effect in ZnO Nanowires, CHUNG-JEN CHIEN, PAI-CHUN CHANG, ZHIYONG FAN, JIA GRACE LU, University of Southern California, DANIEL STICHENTOOTH, CARSTEN RONNING, University of Goettingen, Germany — In this talk, we present electrical and optical measurements on ZnO nanowires whose sizes do not yet reach quantum confinement region. Thin ZnO nanowires were synthesized via carbon thermal chemical vapor deposition method under low growth temperature using tin as catalyst. Electron microscopy reveals that the as-grown nanowires are single crystalline and nanowires' diameter quality with an average diameter around 12 nm. Electrical transport measurements show significant increase in conductivity with a lack of gate modulation and a reduction in mobility. This phenomenon is attributed to the enrichment of surface states owing to the larger surface-to-volume ratio. This enhanced surface effect in thinner nanowires is confirmed by the temperature dependent photoluminescence measurements. In addition, the photoluminescence spectra clarify the apparent blue shift observed at room temperature with respect to the nanowires with larger diameters. These results provide a fundamental insight into nanowires of smaller diameters, and show that their surface states are extremely important and should be properly tailored or controlled for further device applications.

Electrical and Photocooperative Properties of Vertical ZnO Nanowires in High Density Arrays

3:30PM W31.00006 Electrical and Photocooperative Properties of Vertical ZnO Nanowires in High Density Arrays, ZHIYONG FAN, DEEPANSHU DUTTA, CHUNG-JEN CHIEN, EVAN C. BROWN, PAI-CHUN CHANG, JIA GRACE LU, University of Southern California, CALIFORNIA. High density vertical arrays of ZnO nanowires were synthesized using highly ordered channels in anodic alumina membranes (CVD) approach via catalytic chemical vapor deposition method to characterize the morphology growth axis and lattice constant of these materials. The nanowire arrays were grown using a two-step anodization method. High resolution transmission electron microscopy and energy dispersive x-ray microanalysis studies revealed that the nanowire growth was governed by a vapor-liquid-solid mechanism, and the nanowires are single crystalline grown along the [001] direction. Using conductive atomic force microscopy (AFM), the electrical transport and photoconductivity of individual vertical nanowires were investigated. The role of the AFM probe coating on the I – V characteristics was observed as a result of electron tunneling through the alumina membrane due to its high quality layer. In contrast, positive photoconductivity was observed using a thermally annealed anodic alumina membrane as the nanowire growth template. These studies render a pathway for constructing high density nanoscale electronic and optoelectronic circuits.

Imaging the response of individual carbon nanotubes to polarized light in aqueous environments

3:42PM W31.00007 Imaging the response of individual carbon nanotubes to polarized light in aqueous environments, BRYANT WALKER, NIST, Gaithersburg, MD, TODD BRINLINGTER, Dept. of Materials Sci. and Eng., Univ. of Maryland, College Park, MICHAEL S. FUHRER, Dept. of Physics and Center for Superconductivity Research, Univ. of Maryland, College Park, JOHN CUMINGS, Dept. of Materials Sci. and Eng., Univ. of Maryland, College Park, ERIK HOBBIE, NIST, Gaithersburg, MD — Individual carbon nanotubes are grown using chemical vapor deposition (methylene-ethylene carrier gas and iron nitrate catalyst), freely suspended in an aqueous solution using a surfactant (sodium dodecyl sulfate), and imaged in an optical microscope using either fluorescent dye (PKH67 and PKH23) or intrinsic near-infrared fluorescence. Freely suspended, individual carbon nanotubes of length 1-8 micrometers show an increasing response to illuminating light as the polarization becomes parallel to tube axis. More intriguingly, some of the carbon nanotubes are found to collapse and fold under 10-30 seconds of illumination, with increasing tube length showing longer time-to-collapse. Unperturbed persistence lengths in these nanotubes are estimated to be 200-300 micrometers.

Raman spectroscopic investigation of the confined optical phonon modes in the aligned CdSe nanorod arrays

3:54PM W31.00008 Raman spectroscopic investigation of the confined optical phonon modes in the aligned CdSe nanorod arrays, CONCETTA NOLIBE, LUIGI CARBONE, STEFAN KUDERA, LIBERATO MANNA, ROBERTO CINGOLANI, ROYMAR KRABNE, National Nanotechnology Laboratory, VLADIMIR A. FONOBEROV, ALEXANDER A. BALANDIN, University of California — Riverside, GERWIN CHILLA, TOBIAS KIPP, DETLEF HEITMANN, University of Hamburg — Nanocrystal rods have emerged as promising nanostructured material for both fundamental studies of nanoscale physics and for optical and electronic device applications. We investigated the optical phonon excitations in laterally aligned CdSe nanocrystal rod arrays using resonant Raman scattering. Electric-field mediated alignment between interdigitated electrodes has been used to prepare the samples. We report Raman experiments that probe the optical lattice vibrations in ordered arrays of CdSe nanorods with respect to the nanorod orientation. The packing of nanorods into dense arrays leads to the suppression of the surface optical phonon modes. In the longitudinal-optical phonon peak we observe a fine structure that depends on the relative orientation of the nanorods with respect to the incident light polarization. Detailed comparison of the experimental data with the first-principle calculations for corresponding nanostructures, which reveal the symmetry of the phonon potentials for the Raman active modes, provides a qualitative explanation of the experimentally observed phonon modes.

Raman Scattering from Si<sub>1-x</sub>Ge<sub>x</sub> Alloy Nanowires

4:06PM W31.00009 Raman Scattering from Si<sub>1-x</sub>Ge<sub>x</sub> Alloy Nanowires, QIJIE LU, KOFI ADU, Department of Physics, The Pennsylvania State University, XI ZHANG, KOK-KEONG LEW, PRAMOD NIMMATOORI, Department of Materials Sciences, The Pennsylvania State University, ELIZABETH DICKEY, JOAN REDWING, Department of Materials Sciences, Materials Research Institute, The Pennsylvania State University, PETER EKLUND, Department of Physics, Department of Materials Sciences, Materials Research Institute, The Pennsylvania State University — Bulk Si<sub>1-x</sub>Ge<sub>x</sub> crystals can be prepared over a wide composition range 0<x<1. These materials are of interest because alloying can be used to vary the bandgap of the system. Here we present Raman scattering results on Si<sub>1-x</sub>Ge<sub>x</sub> nanowires (0<x<1) grown by the vapor-liquid-solid growth mechanism using a Chemical Vapor Deposition (CVD) approach. The nanowires were grown at 800°C in an iron nitrate catalyst using methane-ethylene carrier gas and are single crystalline grown along the [001] direction. Using conductive atomic force microscopy (AFM), the electrical transport and photoconductivity of individual vertical nanowires were investigated. The role of the AFM probe coating on the I – V characteristics was observed as a result of electron tunneling through the alumina membrane due to its high quality layer. In contrast, positive photoconductivity was observed using a thermally annealed anodic alumina membrane as the nanowire growth template. These studies render a pathway for constructing high density nanoscale electronic and optoelectronic circuits.

Transport and optical properties of electrochemically fabricated Bi nanowires

4:18PM W31.00010 Transport and optical properties of electrochemically fabricated Bi nanowires, HONG ZHANG, HAIĐONG LIU, ZUXIN YE, WENHAO WU, SERGUEI JEREBSKOV, ALEXANDRE KOLOMENSKI, HANS SCHUSSLER, Texas A&M University — We present transport and optical studies of Bi nanowires electrochemically deposited into porous aluminum oxide (AAO) membranes. The Bi wires have nominal diameters of 20-100 nm and length of 60 µm. For transport measurements, electric contacts with negligible contact resistance were formed on single Bi nanowires in-situ during electrochemical deposition. The temperature dependence of the resistance of Bi single nanowires in AAO showed a semiconductor-semimetal transition when the samples were cooled below 50 K. The transverse magnetoresistance increases monotonically up to the highest available field of 8 T, while the longitudinal magnetoresistance tends to flatten at high field values. For optical measurements we first etched away the membranes and suspended Bi nanowires in water and then collected Bi nanowire on glass substrates. Coherent optical phonons were studied in Bi nanowires using a femtosecond pump-probe technique. The frequency of the excited phonon oscillations was found to be 2.35 THz at a pump fluency of 10 mJ/cm².

Dispersion of single-wall carbon nanotubes (SWNTs) in water is critical for processing. Dispersions are often unstable and the dynamics associated with SWNT bundle formation are poorly understood. We have devised a simple method to examine the dispersion characteristics will be presented. A negative photoconductivity was first observed as a result of electron trapping in the alumina membrane due to the illumination of light as the polarization becomes parallel to tube axis. More intriguingly, some of the carbon nanotubes are found to collapse and fold under 10-30 seconds of illumination, with increasing tube length showing longer time-to-collapse. Unperturbed persistence lengths in these nanotubes are estimated to be 200-300 micrometers.

Transport and optical properties of electrochemically fabricated Bi nanowires

4:18PM W31.00010 Transport and optical properties of electrochemically fabricated Bi nanowires, HONG ZHANG, HAIĐONG LIU, ZUXIN YE, WENHAO WU, SERGUEI JEREBSKOV, ALEXANDRE KOLOMENSKI, HANS SCHUSSLER, Texas A&M University — We present transport and optical studies of Bi nanowires electrochemically deposited into porous aluminum oxide (AAO) membranes. The Bi wires have nominal diameters of 20-100 nm and length of 60 µm. For transport measurements, electric contacts with negligible contact resistance were formed on single Bi nanowires in-situ during electrochemical deposition. The temperature dependence of the resistance of Bi single nanowires in AAO showed a semiconductor-semimetal transition when the samples were cooled below 50 K. The transverse magnetoresistance increases monotonically up to the highest available field of 8 T, while the longitudinal magnetoresistance tends to flatten at high field values. For optical measurements we first etched away the membranes and suspended Bi nanowires in water and then collected Bi nanowire on glass substrates. Coherent optical phonons were studied in Bi nanowires using a femtosecond pump-probe technique. The frequency of the excited phonon oscillations was found to be 2.35 THz at a pump fluency of 10 mJ/cm².

Suspension of SWNTs in water: a dynamic optical study

4:30PM W31.00011 Suspension of SWNTs in water: a dynamic optical study, GOKI EDA, GIOVANNI FANCHINI, MANISH CHHIMALA, Rutgers University — Dispersion of single-wall carbon nanotubes (SWNTs) in water is critical for processing. Dispersions are often unstable and the dynamics associated with SWNT bundle formation are poorly understood. We have devised a simple method to examine the dispersion characteristics will be presented. A negative photoconductivity was first observed as a result of electron trapping in the alumina membrane due to the illumination of light as the polarization becomes parallel to tube axis. More intriguingly, some of the carbon nanotubes are found to collapse and fold under 10-30 seconds of illumination, with increasing tube length showing longer time-to-collapse. Unperturbed persistence lengths in these nanotubes are estimated to be 200-300 micrometers.
4:42PM W31.00012 Optical Properties of Nanostructured of Ce-doped Y₂SiO₅; 1. Luiz G. Jacobsohn, Bryan L. Bennett, Ross E. Muenchhausen, James F. Smith, Stephanie C. Sitarz, Michael W. Blair, D. Wayne Cooke, Los Alamos National Laboratory — Nanophosphors correspond to nanostructured inorganic insulator materials that emit light under particle or electromagnetic radiation excitation. In this work, we present structural and optical characterization of Ce-doped Y₂SiO₅ nanophosphor prepared by the solution combustion method. Characterization by TEM and x-ray diffraction shows that nanophosphors are composed of 30-70 nm nanocrystals agglomerated into micron-sized particles. The Ce content was varied up to 10 at.%. Photoluminescence excitation and emission spectra are composed of two major bands centered at 360 and 430 nm, respectively. These results revealed larger Stokes shift for the nanophosphors when compared to bulk. Ce content was also found to affect photoluminescence emission intensity and lifetime. Concentration quenching curve presents a broad maximum centered at 1 at.%. Lifetime measurements showed a continuous decrease from 34 to 21 ns for higher Ce contents. These results confirm the uniqueness nature and properties of nanophosphors, and show that nanophosphors are promising materials for new basic science and technological applications.

1Support by the DOE, Office of Basic Energy Sciences, and by LANL.

4:54PM W31.00013 Optical Properties of Molecular Dots; Timothy Russin, Gugang Chen, James Adair, Peter Eklund, The Pennsylvania State University — A “Molecular Dot” (or “M-dot”) refers to a mixed organic/inorganic phase of nanomatter where a small number of organic molecules are encapsulated in an inorganic nanoparticle. Particular interest has been initiated in these systems when the molecules exhibit photoluminescence (PL) and the nanoparticle provides a transparent medium allowing easy entrance and exit of photons. They show promise for medical applications. In preliminary experimental studies, the encapsulation has been found to enhance the PL and suppress the photo-degradation of organic dye molecules such as Rhodamine B encapsulated in SiO₂ or CaPO₄. In this paper, we present the results of an optical model to predict the optical properties of M-dots. Using the discrete dipole approximation, we take into account the effects of Mie scattering and the effective dielectric function of the dye molecules encapsulated in an inorganic host of known refractive index. The results of the modeling will be compared to recent experimental results on M-dots in dilute solution, i.e., optical absorption and dispersion in the NIR-Vis-UV regions.

1Department of Physics
2Department of Material Sciences
3Department of Physics, Department of Material Sciences


5:18PM W31.00015 Second-Harmonic Generation of Aligned Single-Walled 0.4nm Carbon Nanotubes; KAM SING WONG, HUIMIN SU, JIANTING YE, ZIKANG TANG, The Hong Kong University of Science and Technology — The second-harmonic generation (SHG) is measured for the first time from monosized and well-aligned single-walled carbon nanotubes (SWCNT) in the channel of aluminophosphate AIP04-5 (AFI) zeolite. The SHG yield scales as quadratic function of the pump laser intensity. Due to the different polarization preference, we are able to discriminate the SHG contribution from the chiral (4,2) CNTs and those from the AFI template. The polarization direction and the anisotropic dependence of the SHG intensity on the excitation polarizations are investigated in the transmission geometry. In the case of normal incidence, the intensity of SHG is maximized when the excitation polarization is 45 degree against the tube axis and the SH radiation is linear-polarized on the plane perpendicular to the tube axis. The experiment results are in excellent agreement with the theoretical prediction of the second-order nonlinear optical process in chiral carbon nanotubes. 1

5:30PM W31.00016 Monolayer Degradation and Sidewall Tribometer Studies of Vapor Phase Lubricants for MEMS; 1. Daniel Adam Hook, Brendan Miller, North Carolina State University, Shannon J. Timpe, University of California at Berkeley, Michael T. Dugger, Sandia National Laboratories, Jacqueline Krim, North Carolina State University — Monolayers have been widely used for MEMS to prevent release related stiction as well as adhesion as the devices are stored for long periods of time. Degradation of these monolayers in mechanical contact and at elevated temperatures however render the devices useless after a short period of time. While vapor-phase lubricants have primarily been studied within the context of macroscopic system performance, they may ultimately prove to be the most effective, if not the only, means to deliver and/or replenish a lubricant that can withstand a variety of extreme environmental conditions that a MEMS device is likely to encounter. We have made direct measurements of the change in the coefficient of friction of a MEMS sidewall tribometer as the lubricant is added to a vacuum chamber. Monolayer degradation under normal contact, requirements to prevent device failure, and friction measurements of vapor phase lubricants will be presented.

1Work funded in part by Sandia National Labs MESA Project and the AFOSR Extreme Friction MURI.

Thursday, March 8, 2007 2:30PM - 5:06PM — Session W42 DCMP: Liquids and Tribology Colorado Convention Center 505

2:30PM W42.00001 Monolayer Degradation and Sidewall Tribometer Studies of Vapor Phase Lubricants for MEMS; Daniel Adam Hook, Brendan Miller, North Carolina State University, Shannon J. Timpe, University of California at Berkeley, Michael T. Dugger, Sandia National Laboratories, Jacqueline Krim, North Carolina State University — Monolayers have been widely used for MEMS to prevent release related stiction as well as adhesion as the devices are stored for long periods of time. Degradation of these monolayers in mechanical contact and at elevated temperatures however render the devices useless after a short period of time. Vapor-phase lubricants have primarily been studied within the context of macroscopic system performance, they may ultimately prove to be the most effective, if not the only, means to deliver and/or replenish a lubricant that can withstand a variety of extreme environmental conditions that a MEMS device is likely to encounter. We have made direct measurements of the change in the coefficient of friction of a MEMS sidewall tribometer as the lubricant is added to a vacuum chamber. Monolayer degradation under normal contact, requirements to prevent device failure, and friction measurements of vapor phase lubricants will be presented.
3:42PM W42.00002 Tribological properties of bound plus mobile lubricants for MEMS application. BRENDA MILLER, D. ADAM HOOK, JACQUELINE KRAM, North Carolina State University, AFOSR MURI EXTREME FRICTION TEAM. Long chain alkylsilane monolayers are used to protect MEMS devices from adhesion due to contamination. One such monolayer, perfluorodecytrichlorosilane (PFTS) has been shown to have very advantageous thermal properties but will wear under mechanical rubbing. The mobility of vapor phase lubricants (VPL) used in conjunction with these self-assembled monolayers (SAMs) may be the key to extending the lifetime of rubbing contacts in MEMS by replenishing worn away parts of the SAM. We studied tricresyl phosphate, a known anti-oxidant, and Nyme lubricant, used for aerospace applications. We measured friction and obtained wear characteristics with a quartz crystal microbalance (QCM), a sliding tribometer under cryogenic temperatures, and an AFM in order to understand the effect of mobility, temperature, and atomic-point contacts to help bridge the gap between fundamental friction and MEMS application.

3:42PM W42.00003 Self-organization of surfactant aggregates on rough and smooth surfaces HANNES C. SCHNIEPP, Chemical Engineering Department, Princeton University, HO C. SHUM, DUDLEY A. SAVILLE, ILHAN A. AKSAY, CERAMIC MATERIALS LABORATORY TEAM. Atomic force microscopy (AFM) investigations of surfactant aggregates at liquid-solid interfaces have traditionally been performed on atomically smooth mica, graphite or gold. In order to extend the utility of this technique to more practical applications where atomically smooth surfaces rarely exist, we present results on rough gold surfaces for the first time. We achieve high-quality images of micellar structures on rough surfaces by using sharp, soft AFM probes. Contrary to the orientational order observed on atomically smooth surfaces, micellar organization on rough surfaces is also affected by the grain boundaries and atomic ledges. Our approach opens up the possibility of investigating surfactant self-assembly on arbitrary materials.

3:06PM W42.00004 Real-time observation of self-assembling nanostructures of Langmuir-Blodgett films of vinylidene fluoride-trifluoroethylene copolymer by Atomic Force Microscopy. JHEE KIM, STEPHEN DUCHARM, Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588-0111, BRIAN RODRIGUEZ, SERGEI KALININ, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831. Annealing studies have shown that ferroelectric polymer Langmuir-Blodgett (LB) films less than 10 nm thick undergo drastic morphology change after annealing in the crystalline ferroelectric phase [M. Bai et al., Appl. Phys. Letts. 85, 3528 (2004)] During annealing in the crystalline paraelectric phase, continuous films self-assemble into disk-shape features, nanomesas, with approximately 9 nm thickness and 100 nm diameter. The nanomesa self-assembly was observed in real time with an Atomic Force Microscope, which was equipped with a heating stage. This results show that the nanomesas formed during annealing agree well with nanomesas observed in ferroelectric phase at room temperature after annealing in the paraelectric phase.

3:18PM W42.00005 Study of Low Temperature Fuel Cells Thin Films Morphology by GISAXS TOMOMI IRITA, THOMAS RUSSELL, University of Massachusetts — Grazing incidence small angle x-ray scattering experiments were performed on thin films of Nafion solutions as a function of time as the solvent, methanol/water, evaporated. The development and orientation of the structure and morphology in the thin films, at the free surface and in the bulk of the film, was characterized by the scattering below and above the critical angle. The scattering profiles indicated that Nafion thin morphology was strongly influenced by the conformations of Nafion molecules in the solutions. In addition, the morphology in thin films of sulfonated block copolymers of polystyrene-b-poly(ethylene-o-butylene)-b-polystyrene, an alternative material for fuel cell applications, was characterized by GISAXS and scanning force microscopy using optical and applied electric fields. Both the solvents used and the applied field was found to markedly influence the orientation of the ion conducting domains in the films.

3:30PM W42.00006 Feasibility of Large Free-standing Liquid Films in Space RUI ZHENG, THOMAS WITTEN, James Franck Institute and Department of Physics, University of Chicago — We consider the feasibility of large-scale free-standing thin liquid film experiment in the space environment as a new realization to study two-dimensional hydrodynamics. We identify material and environmental criteria necessary to avoid freezing, evaporation, chemical degradation, and spontaneous collapse of the film. These criteria pose no obstacles to achieving films of kilometer scale and lifetime of many months, with attainable Reynolds number up to $10^7$. However, impacts from meteoroids pose a serious threat to the film, and require substantial shielding or unproven self-healing properties in the film. Current theoretical and experimental studies of two-dimensional turbulence are briefly reviewed. We also describe a specific candidate liquid for the film.

3:42PM W42.00007 Characterization of Surface Nanobubbles SHANGJIONG YANG, STEPHAN DAMMER, HAROLD ZANOVIET, STEFAN KOOLJ, BENE POELSEMA, DETLEF LOHSE, Physics of Fluids, University of Twente, PHYSICS OF FLUIDS, UNIVERSITY OF TWENTE TEAM, SOLID STATE PHYSICS, UNIVERSITY OF TWENTE COLLABORATION. In this work we characterize surface nanobubbles on hydrophilic surface in water by Atomic Force Microscopy (AFM) operated in the tapping mode. A connection between the formation of nanobubbles and the surface topography is presented. Together with large contact angle of nanobubbles, which determines their shape, the surface topology may support the surfactant stability of nanobubbles. It is shown that the properties of the nanobubbles and their density are sensitive to the gas concentration and type. We show that different surface treatments also influence nanobubbles in formation and shape. Next, adding surfactants (2-butanol) causes nanobubbles to shrink, as expected from the Laplace equation. Finally, we show that exchanging alcohols by water on the surface strongly encourages the formation of nanobubbles.

3:54PM W42.00008 High Density Monolayer Deposition of Fine Nanoparticles for Opto-Electronic Devices XAVIER BULLIARD, WANKI BAE, KOOKHEON CHAR, School of Chemical and Biological Engineering, NSI-NCRC, Seoul National University, Seoul, Korea, SEONG JAE CHOI, JAE YOUNG CHOI, Display Device and Material Lab., Samsung Advanced Institute of Technology. In this study, we presented a unique approach to form uniform monolayers of nanoparticles (NPs) deposited on a substrate with high surface coverage density up to $2 \times 10^{12}$ NPs/cm$^2$. This was achieved through the wet coating of fine NPs with a diameter less than 10 nm. The mechanism of monolayer formation was decomposed into two stages: first the deposition driven by the electrostatic forces between a substrate and NPs and then the self-arrangement of NPs through the action of capillary forces. A physical description of the interaction forces involved in the process confirmed that for fine NPs the capillary forces are dominant over the electrostatic repulsion between adjacent NPs during drying. This enables the high compaction of a monolayer without altering its uniformity. Dip- and spin-coating techniques could as well be used for the deposition on various substrates (for example, hafnium and silicon oxides), which proves the versatility of this approach. The obtained architecture show promising properties and could be implemented for the production of the next generation of opto-electronic devices.
4:06PM W42.00009 Microcontact printing Using Metallic Salt Solution “Ink”

CARY ALLEN, JOSH DORR, IAN SCHICK, EVAN SCHICK, REUBEN COLLINS, Colorado School of Mines, ANISH KHANDEKAR, THOMAS KUECH, University of Wisconsin-Madison — Arrays of micron size metal dots were patterned onto Si substrates using microcontact printing. Poly(dimethylsiloxane) stamps were prepared from Si masters fabricated using photolithography and anisotropic etching. Aqueous GaCl₃ and In(NO₃)₃ inks were microcontact printed onto Si substrates, creating arrays of micron size metal salt deposits. The In(NO₃)₃ deposits were further processed by annealing in an N₂:H₂ (9:1) forming gas environment at 600 °C which converted the deposits into In metal. Details of the stamp preparation and printed patterns, along with, characterization using atomic force microscopy and X-ray diffraction will be presented. The ability to inexpensively pattern metal arrays on semiconductor surfaces has implications for ohmic contacts and, with additional processing, arrays of semiconductor crystalstallites for optoelectronic applications.

1Work supported by the National Science Foundation and Air Force Research Laboratory.

4:18PM W42.00010 X-ray diffuse scattering from thin polystyrene films

MRINMAY K. MUKHOPADHYAY, ZHANG JIANG, SUNIL K. SINHA, University of California, San Diego, CA 92093, LAURENCE B. LÚRIO, JARETT STARK, Northern Illinois University, DeKalb, IL 60115, XUESONG JIAO, SURESH NARAYANAN, ALEC SANDY, Advanced Photon Source, Argonne, IL 60439 — Diffuse x-ray scattering from silicon supported polystyrene films has been measured as a function of thickness. An x-ray standing wave method was used to distinguish scattering from the surface and scattering from density fluctuations within the interior of the film. The former is a measure of surface roughness, while the latter yields the compressibility, υ. Films thicker than h ≈ 100 nm had bulk values for υ, while thinner films showed the empirical relation υ(h) = υbulk(1 + α|h|) with α = 20 (±1) nm and δ = 1.6 ± 1. The surface component of the scattering agreed with capillary wave theory for small q, but excess scattering appeared at larger q, which followed a power law, S ∼ q¹/v. We attribute the excess scattering to static roughness from chain ends and loops near the surface.

4:30PM W42.00011 ABSTRACT WITHDRAWN —

4:42PM W42.00012 New Cyclic Voltammetry Method for Examining Phase Transitions on Electrodes: Simulated Results

IBRAHIM ABOU HAMAD, DANIEL ROBB, PER ARNE RIKVOLD, Florida State University, Tallahassee, FL 32310 — We propose a new experimental technique for cyclic voltammetry, based on the first-order reversal curve (FORC) method for analysis of systems undergoing hysteresis. The advantages of this technique are demonstrated by applying it to dynamical models of electrochemical adsorption. The method can not only differentiate between discontinuous and continuous phase transitions, but can also quite accurately recover equilibrium behavior from dynamic analysis of systems with a continuous phase transition. The FORC diagram for a discontinuous phase transition is characterized by a negative (unstable) region separating two positive (stable) regions, while such a negative region does not exist for continuous phase transitions. Experimental data for Electrochemical FORC (EC-FORC) analysis could easily be obtained by simple reprogramming of a potentiostat designed for conventional cyclic-voltammetry experiments.


4:54PM W42.00013 Relating contact angles, drop size and Line Energy

PREETI YADAV, PRASHANT BAHADUR, KUMUD CHAURASIA, RAFAEL TAMGOR, Lamar University — The relation between drop radius, r, the force to slide it, and the advancing and receding contact angles, θA and θR, has been studied. To keep the line energy (energy per 2πr) independent of r, the modified Young equation predicts that θA and θR change considerably with r. As shown by many investigators, θA and θR change negligibly, if at all, with r. We show why the modified Young equation is correct and still θA and θR should hardly change with r. Our results suggest that the Laplace pressure is a significant parameter in inducing the line energy.

Thursday, March 8, 2007 2:30PM - 5:18PM –
Session W43 DCMP: Coupled 2D and Multiple Quantum Dot Systems

Colorado Convention Center 506

2:30PM W43.00001 A study of interminiband Rabi oscillations in biased semiconductor superlattices

PAVEL ABUMOV, DONALD SPRUNG, Dept. of Physics and Astronomy, McMaster University, Hamilton ON L8S 4M1, Canada — Semiconductor superlattices can be a flexible source of coherent electrons, with possible application as sources of terahertz radiation and in quantum computing. A better understanding of the underlying quantum transport phenomena is essential for making further progress in these fields. We have studied interminiband Rabi oscillations of an electron in biased semiconductor superlattices, specifically the conditions for their occurrence and their variation with bias tuning at energy level anticrossings. Our simulations were based on direct solution of the time-dependent Schrödinger equation, using transparent boundary conditions. It has been explicitly demonstrated that interminiband Rabi oscillations result from constructive interference between Bloch and intrawell oscillations, and the conditions for resonant bias values have been investigated. We also report a simulation of interminiband Rabi oscillations directly across three minibands at high bias, which show interaction between three strongly coupled minibands.

1Work supported under NSERC discovery grant RGPIN-3198.

2:42PM W43.00002 Microwave Switching in Amorphous-Carbon Quantum Wells

SOMNATH BHAT-TACHARYYA, LUIS GOMEZ ROJAS, S. RAVI, P. SILVA, Nano-Electronics Centre, Advanced Technology Institute, University of Surrey, Guildford, GU2 7XH, UK — Demonstration of long phase coherence length showing resonant tunnelling and fast switching in amorphous carbon quantum well structures has recently been established [1]. Here we show a bias controlled reversible switching of the complex impedance by transmitting a microwave signal up to 110GHz through amorphous carbon resonant tunnel diodes. By employing a coplanar waveguide technique and through the analysis of the return loss (S₁₁) microwave enhanced mobility greater than 30cm²/Vs in the delocalized regime of (filamentary) conduction in these devices is demonstrated. Also a switching behaviour at about 85GHz can also be observed. We suggest a new model for the microscopic origin of the increased mobility and show routes to achieve longer coherence lengths. In addition microwave conductance of carbon quantum wells parallel to their plane and across a channel length larger than 100 nm determines the momentum scattering time of electrons in carbon. These results exhibit a potential for pure amorphous carbon-based fast memory devices. [1] S. Bhattacharyya, S.J. Henley, E. Mendoza, L. Gomez Rojas, J. Allam and S.R.P. Silva, Nature Mater. 5, 19 (2006).
2:54PM W43.00003 Transient response and electric field domain relocation in semiconductor superlattices, HUIDONG XU, STEPHEN TEITSWORTH, Duke University — Numerical simulation results are presented for a discrete drift-diffusion model that describes electronic transport in weakly-coupled semiconductor superlattices under voltage bias [1]. Sequential resonant tunneling between adjacent quantum wells is the primary conduction mechanism for this model which also incorporates an effective conductivity \( \sigma \) associated with the injecting contact. We study time-averaged current-voltage characteristics and the transient current response associated with electric field domain relocation when the applied voltage is abruptly shifted by an amount \( V_{\text{step}} \). For intermediate values of \( \sigma \) and a range of \( V_{\text{step}} \) values, two types of complex transient response are observed: 1) the tripole/dipole mechanism in which a charge depletion and a charge accumulation layer move together from the contact, and 2) the injected monopole mechanism, in which a small amplitude accumulation layer moves rapidly from the contact. Generally, the injected monopole relocation mechanism is much faster than the tripole/dipole mechanism. At moderately larger values of \( \sigma \), the tripole/dipole mechanism is not observed for any value of \( V_{\text{step}} \), because the higher levels of injected charge suppress formation of a moving depletion layer. Thus, a relatively small increase in \( \sigma \) can result in significantly shorter domain relaxation times. [1] L. L. Bonilla and H. T. Grahn, Rep. Prog. Phys. 68, pp. 577 - 683, and references therein.

3:06PM W43.00004 Exchange-driven re-entrant layer-occupancy transitions in biased bilayer systems, J.R. RODRIGUEZ, C.B. HANNA, Boise State University — Hamilton et al. showed experimentally that an externally biased double-quantum-well system in zero magnetic field could exhibit an exchange-driven bilayer-to-monolayer (“2-1”) transition as the total carrier density was increased. This transition is due to the combined effects of the negative compressibility of the low-density carriers and the layer imbalance produced by external gate biases. We give an approximate criterion for observing a re-entrant “2-1-2” transition that repopulates the emptied layer as the total carrier density is further increased. The gate voltages required for repopulation are shown to be impractically high for \( n \)-type GaAs bilayer devices with hole carriers. We show, however, that it may be possible to observe a “2-1-2” transition in low-density \( n \)-type electron bilayer systems with very small layer separations.

3:18PM W43.00005 Using the angular dependence of a quantizing magnetic field to probe the Bloch states in room temperature superlattice devices, ROSS MCDONALD, Los Alamos National Lab., SHIGEKI KOBAYASHI, S. JIM ALLEN, UCSB, SUSAN COX, JOHN SINGLETON, LANL — The prospect of designing Bloch-oscillator superlattice structures that operate at room temperature has both intrigued and eluded the scientific community since its conception over 35 years ago. Advances in band structure architecture and engineering continuously address this issue, improving the fabrication of devices designed to operate as room temperature THz frequency oscillators. Here we report room-temperature pulsed-IV measurements in tilted magnetic fields of up to 30 Tesla, designed to probe the coherence of superlattice Bloch states. Biasing these devices beyond Ohmic conduction reveals differential conductance features with a 1/(\cos(\theta)) dependence upon the field angle. The voltages at which these features occur is determined by the condition that the ratio of the Bloch to cyclotron frequencies be an integer. This behavior is consistent with resonant de-localization of Bloch oscillations due to nonlinear coupling to the cyclotron motion in tipped field.

3:30PM W43.00006 Effective Hamiltonian Approach for the Magnetic Band Structure and Novel Oscillations in the Magnetization, MANFRED TAUT, Leibniz Institute for Solid State and Materials Research, Dresden, Germany — The one-electron Schrödinger equation in a 2D periodic effective potential and an homogeneous magnetic field \( B \) has been solved numerically in the framework of magnetic band structure theory. Alternatively, the spectrum around a given rational flux quantum number \( p_0/q_0 \) can also be obtained by using semi-classical quantization of the exact magnetic band structure (MBS) at \( p_0/q_0 \). To implement the latter procedure, a generalized effective Hamiltonian theory based on the MBS at finite magnetic fields has been established. The total energy has been calculated numerically as a function of magnetic field \( B \) and of band filling. The magnetization \( M \) is the derivative of the total energy with respect to the magnetic field. The total energy as a function of magnetic field \( B \) shows series of kinks, which produce series of oscillations in the magnetization. One of these series, the de Haas-van Alphen oscillation, contains information about the (zero magnetic field) band structure. The other series provide the corresponding information about certain MBSs. In order to obtain the information about the MBS at field \( B \), we have to plot the magnetization as a function of \( 1/(B-B_0) \). The asymptotic period of the oscillations in \( M(1/(B-B_0)) \) provides the Fermi surface cross sections for the MBS at \( B_0 \).

3:42PM W43.00007 Novel Flux Matching Effects in Potentially Type-I Superconducting Au/Pb Bilayers Patterned with Antidot Lattices, LANCE DE LONG, SERGIY KRYUKOV, University of Kentucky, VI-TALI METLUSHKO, University of Illinois-Chicago — We report AC and DC SQUID magnetometer data for Au(25nm)/Pb(x) bilayers (x = 50, 100 nm) patterned with square antidot (AD) lattices having AD diameter \( D = 600 \) nm and AD separation \( d = 1 \) micron, in DC magnetic fields applied perpendicular to the film plane. Both AC and DC data for \( x = 100 \) nm samples exhibit a “two-horned” magnetization \( m(\mathbf{H}) \) well below \( T_C \), with small, sharp cusps having DC fields spacings near \( 3 \) Oe. Just below \( T_C = 6.2 \) K, \( m(\mathbf{H}) \) is highly reversible, and exhibits at least two matching fields \( H_m = (20 \text{ Oe})/n \). This striking behavior is compared with recent theoretical models for flux matching in patterned films in the Type-I intermediate state, for which formation of “giant vortices” or pinning of normal domains by AD is possible. In contrast, for data \( x = 50 \) nm samples exhibit smooth (no small cusps) \( m(\mathbf{H}) \) behavior with sharp matching peaks and highly irreversible behavior just below \( T_C \), typically of extensively studied, Type-II patterned films.

3:54PM W43.00008 Variational Monte Carlo Method for Coupled Quantum Dots in Magnetic Fields, J.IHAN KIM, DMITRIY MELNIKOV, MICHELE CASULA, JEAN-PIERRE LEBURTON, University of Illinois at Urbana-Champaign — The electronic properties of two-dimensional coupled quantum dots (QD) in presence of an external magnetic field are investigated using a variational Monte Carlo (VMC) method. The many-body Schrödinger Equation with fixed model potential for coupled QDs is solved by using two-electron trial wavefunctions made of a product of two-body Jastrow term and single-particle orbitals for both singlet and triplet states. We use the steepest descent (SD) method to optimize the expectation value of energy by iteratively updating the variational parameters. In co-linear triple QDs, we show that the exchange energy between two electrons can be tuned by varying the confinement of the central dot. We also find that the electron separation in the singlet and triplet states evolve differently upon increasing the magnetic field.

1Supported by NSF DMR-0206681 and by the Research Corporation.

3:54PM W43.00008 Variational Monte Carlo Method for Coupled Quantum Dots in Magnetic Fields, J. IHAN KIM, DMITRIY MELNIKOV, MICHELE CASULA, JEAN-PIERRE LEBURTON, University of Illinois at Urbana-Champaign — The electronic properties of two-dimensional coupled quantum dots (QD) in presence of an external magnetic field are investigated using a variational Monte Carlo (VMC) method. The many-body Schrödinger Equation with fixed model potential for coupled QDs is solved by using two-electron trial wavefunctions made of a product of two-body Jastrow term and single-particle orbitals for both singlet and triplet states. We use the steepest descent (SD) method to optimize the expectation value of energy by iteratively updating the variational parameters. In co-linear triple QDs, we show that the exchange energy between two electrons can be tuned by varying the confinement of the central dot. We also find that the electron separation in the singlet and triplet states evolve differently upon increasing the magnetic field.

1Work supported by the Material Computational Center under NSF Grant 0325939.
4:06PM W43.00009 Topological Hunds rules and the electronic properties of a triple lateral quantum dot molecule, P. HAWRYLAK, M. KORKUSINSKI, F. DELGADO, L. GAUDREAU, S. STUDENIKIN, A. KAM, A. SACHRAJDA, Institute for Microstructural Sciences, National Research Council of Canada — We analyze theoretically and experimentally the electronic structure and charging diagram of three coupled lateral quantum dots in a magnetic field filled with electrons. Using the Hubbard model and real-space exact diagonalization techniques we show that the electronic properties of this artificial molecule can be understood using a set of topological Hunds rules[1]. These rules relate the multi-electron energy levels to spin and the inter-dot tunneling t, and control charging energies. We map out the charging diagram for up to N = 6 electrons and predict a spin singlet for two electrons, spin-polarized phase for two holes, and a magnetically frustrated ground state for three electrons. We show that spin polarization can be tuned by magnetic field perpendicular to the triple dot device. The theoretical charging diagram is compared with the measured charging diagram of the gated triple-dot device[1]. [1] P. Hawrylak and M. Korkusinski, Solid State Commun. 136, 508 (2005). [2] L. Gaudreau, S. A. Studenikin, A. S. Sachrajda, P. Zawadzki, A. Kam, J. Lapointe, M. Korkusinski, and P. Hawrylak, Phys. Rev. Lett. 97, 036807 (2006).

4:18PM W43.00010 Tunable Noise Cross-Correlations in a Double Quantum Dot, DOUGLAS MCCLURE, LEONARDO DICARLO, YIMING ZHANG, HANS-ANDREAS ENGEL, CHARLES MARCUS, Harvard University, MICAH HANSON, ART GOSSARD, University of California, Santa Barbara — We report the measurement of the cross-correlation between temporal current fluctuations in two quantum dots in the Coulomb blockade regime, with purely capacitive inter-dot coupling. The dots act as a pair of tunable interacting localized states, enabling a systematic study of Coulomb-induced correlation. The sign of the cross-spectral density is found to be tunable by gate voltage and source-drain bias. We find good agreement between the experimental results and a sequential-tunneling model of transport through capacitively coupled single-level dots.

1We acknowledge support from the NSF through the Harvard NSFEC, PHYS 01-17795, DMR-05-41988, DMR-0501796, as well as support from NSA/DTO and Harvard University.

4:30PM W43.00011 Phonon decoherence in a double dot qubit embedded inside a suspended phonon cavity, YING-YEN LIAO, Department of Electrophysics, National Chiao-Tung University, Hsinchu 300, Taiwan, YUEH-NAN CHEN, National Center for Theoretical Sciences, Tainan 701, Taiwan, DER-SAN CHU, Department of Electrophysics, National Chiao-Tung University, Hsinchu 300, Taiwan — The phonon-induced decoherence in a double dot charge qubit embedded inside a semiconductor slab is investigated theoretically. We employ the Redfield formalism to solve the density matrix in the Born-Markov approximation. Our calculations show some interesting results in the presence of slab cavity. In particular, the decoherence behaves significantly due to particular phonon couplings such as the van Hove singularity and vanishing deformation potential.

4:42PM W43.00012 Investigation of chaos-assisted tunneling in a weakly coupled, double quantum dot, DONG HO WU, Naval Research Laboratory, BERNARD MATIS, Naval Research Laboratory/ Temple University — It is known that chaos-assisted dynamical tunneling may occur in nonintertwined (chaotic) systems. In our previous experiments we measured the tunneling rate in a weakly coupled, 2D microwave double cavity. The results seem to indicate that the presence of chaotic modes changes not only the dynamical tunneling rate but also the spatial tunneling rate, as the electromagnetic-field leakage (wave tunneling) rate between the weakly coupled, 2D double cavities increases significantly if one of the cavities is nonintertwined. We have now investigated these phenomena with gate-defined quantum dots, fabricated on a GaAs/AlGaAs 2DEG substrate. The experiments were performed on quantum dots of various shapes. In this presentation we will discuss these recent results on tunneling rate and quantum conductance.

4:54PM W43.00013 Fermi-liquid versus non-Fermi-liquid behavior in triple quantum dots, JANEX BONCA, FMF, University of Ljubljana, J. Stefan Institute, Ljubljana, Slovenia, ROK ZITKO, J. Stefan Institute, Ljubljana, Slovenia — We study the effect of electron hopping in triple quantum dots modelled by the three-impurity Anderson model. In a wide interval around the particle-hole symmetric point, the triple quantum dot system has a FL ground state with high conductance at T = 0. The different regimes exhibit different approaches to this fixed point. The most likely candidate for observing non-FL behavior is the cross-over regime with competing magnetic ordering and Kondo screening, J ≈ T_K. In this regime the FL behavior occurs in a wide temperature range and it is fairly robust against various perturbations that do not additionally increase the channel asymmetry. As the crossover regime is entered from the above, the conductance through the side dots increases to a half of the conductance quantum, while the conductance through the system remains small. At lower temperatures the conductance through the system increases to the unitary limit as the system crosses over to the FL ground state. The signature of the FL behavior can be detected by measuring different conductances in a three terminal configuration. Our findings suggest, that properly choosing parameters of the triple quantum dot system that set it into the crossover regime, represents a road map for observation of FL behavior.

5:06PM W43.00014 Signatures and Implementations of Adiabatic Quantum Pumping, KUNAL DAS, Fordham University — We explore the mechanism of adiabatic quantum pumping from a fundamental quantum mechanical perspective, and consider analogies with other adiabatic processes. We discuss ideas for generalizing the mechanism to alternate entities other than charge and spin and in alternative physical systems. Our study is motivated by and grounded in possibilities of easier experimental realizations to get around the difficulties encountered in previous mesoscopic experiments. In addition we wish to have an unambiguous definition and signature for the phenomenon of quantum pumping.

Friday, March 9, 2007 8:00AM - 11:00AM__
Session X1 DCMP: Magnetic Field Driven Quantum Phase Transitions Colorado Convention Center Four Seasons 2-3

8:00AM X1.00001 Field-tuned quantum critical points, ACHIM ROSCH, University of Cologne — No abstract available.

8:36AM X1.00002 Dimensionality and Quantum Criticality: the case of the spin-dimer system BaCuSi$_4$O$_6$, SUCHITRA E. SEBASTIAN, Cambridge University — Physical properties in the vicinity of a quantum critical point (QCP) are intimately related to system dimensionality. In heavy fermion systems, for instance, the origin of emergent superconductivity and non Fermi liquid behaviour at a pressure-tuned QCP has been suggested to be a consequence of reduced dimensionality. The field-tuned Bose Einstein condensation (BEC) QCP in the spin-dimer system BaCuSi$_4$O$_6$ - also known as Han Purple. Long-range antiferromagnetic order in this system appears above a critical magnetic field H$_{c1} \approx 23.5$ T due to the closure of the spin gap to triplon excitations. While the divergence of critical fluctuations tends to destabilise any reduction of dimensionality at a fermionic QCP, contrary behaviour is demonstrated at the field-tuned bosonic QCP in BaCuSi$_4$O$_6$. The suppression of amplitude fluctuations at the BEC QCP in this system contributes to the effectiveness of geometrical frustration in reducing the effective dimensionality at the QCP. Experimental thermodynamic signatures are presented as evidence for a 2D BEC QCP in BaCuSi$_4$O$_6$.


9:12AM X1.00003 Fingerprints of Interacting Hardcore Bosons on a Lattice: Spin Dynamics in Dimer Spin Systems with Field-Tuned Quantum Criticality. CHRISTIAN RUEGG, University College London — Spin-dimer based magnetic insulators are model systems for the experimental and theoretical investigation of field-tuned quantum criticality and, in particular, the ground states of strongly interacting hard core bosons (triplets), for which there are increasing parallels to ultra-cold atoms in optical lattices. We have investigated corresponding quantum phase transitions by inelastic neutron scattering (INS) in spin systems, which cover both the effect of dimensionality and the degree of quasi-particle mobility. These quantities characterize the triplet excitations and define the magnon-BEC phases above the field-induced quantum critical point in these materials. Inorganic compounds like the 3D copper-halide family ACuCl3 (A=K, Tl, NH4), the strongly frustrated Shastry-Sutherland material SrCu2(BO3)2, and quasi-2D BaCuSi2O6 all show distinct spin dynamics associated with the boson system, which they represent. The fascinating quasi-1D limit is accessible in novel organic materials, which promote a characteristic quantum phase – the Luttinger spin-liquid. Recent INS results, which explore this exciting quantum phase, will be compared to those obtained in higher dimensions and elaborate predictions by theory.

9:48AM X1.00004 Field-induced magnetism and quantum criticality in superconducting CeRhIn5 under pressure. TUSON PARK, Los Alamos National Laboratory — The antiferromagnet CeRhIn5 becomes superconducting under pressure, where superconducting state coexists with the helical magnetic state with $Q=(0.5, 0.5, 0.293)$. Similarly to other heavy fermion superconductors, however, magnetism disappears when the antiferromagnetic transition temperature becomes equal to superconducting temperature, hiding a magnetic quantum critical point. Applying magnetic field reveals a low-temperature specific heat anomaly in the unconventional superconducting state, which defines a quantum phase transition from a solely superconducting state to a phase with coexisting magnetic and superconducting orders [1]. The field-pressure phase boundary at zero temperature is anticipated theoretically [2] and is strikingly similar to that in high-Tc cuprates [3], delineating a correlation between quantum criticality and unconventional superconductivity.


10:24AM X1.00005 Magnetic-field quantum phase driven transitions in CeBiPt and CeCu$_6$-$_{x}$Au$_x$. HILBERT V. LÖHNEYSEN, Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe — The half-Heussler compounds CeBiPt and LaBiPt are semimetals with very low charge-carrier concentrations as evidenced by Shubnikov-de Haas (SdH) and Hall-effect measurements. Elastic neutron-scattering results reveal a simple antiferromagnetic structure in CeBiPt below $T_N=1.15$ K. The band structure of CeBiPt sensitively depends on temperature, magnetic field, and stoichiometry. Above a certain, sample-dependent, threshold field ($B>25$ T) the SdH signal disappears and the Hall coefficient reduces significantly. These effects are absent in the non-4f compound LaBiPt. Electronic-band-structure calculations can well explain the observed behavior by a 4f-polarization-induced Fermi-surface modification. CeCu$_6$-$_{x}$Au$_x$ orders for $x > 0.1$ with an incommensurate antiferromagnetic structure. Here we compare the magnetic fluctuation spectrum obtained from inelastic neutron scattering for a field-driven quantum phase transition at $x=0.2$ with that for zero-field transition at the critical concentration $x_{c}=0.1$. Work performed in collaboration with J. Wosnitza, G. Goll, A. D. Bianchi, B. Bergk, N. Kozlova, I. Ophale, S. Elgazzar, M. Richter, O. Stockert, T. Yoshino, T. Takabatake and M. Enderle.

Friday, March 9, 2007 8:00AM - 11:00AM — Session X3 DCMP: DNA Organization within Chromosomes Colorado Convention Center Korbel 2A-3A

8:00AM X3.00001 Structure and Dynamics of the Kinetochore. KERRY BLOOM, University of North Carolina — No abstract available.

8:36AM X3.00002 Structural Organization and Properties of DNA in the Cell. DIETER W. HEermann, University of Heidelberg — The dynamical architecture of the cell nucleus can be regarded as one of the “grand challenges” of modern molecular and structural biophysics. The genomic DNA and the histone proteins compacting it into chromosome account for the major part of the content of the nucleus. In my talk I will discuss the structural properties of the DNA from the 30nm fiber up the entire chromosome. For the 30nm range I present a model for the compactification and discuss the resulting phase diagram. I am going to reveal the fine-structure of the excluded-volume borderline. Furthermore, the effect of the Coulomb repulsion of the DNA linkers will be presented. Moving up further in the range (300-800nm), we will look at the entanglements of the polymer chain. On the level of the entire chromosome I will present a model for the chain that can successfully describe experimentally measured distance distributions on chromosome 1 in human cells using the notion of “ridge” regions (cluster of strongly expressed genes) and the “antiridge” regions.

9:12AM X3.00003 Dynamics of Single Molecule DNA. TIMOTHE LIONNET, ENS/Paris — No abstract available.


10:24AM X3.00005 Dynamics of Nucleosome Arrays. MICHAEL POIRIER, Ohio State University — DNA sites wrapped into chromatin are sterically occluded from proteins that must bind for processes such as RNA transcription and DNA repair. However, the role of chromatin compaction in biological function is poorly understood. To understand the biological functions of chromatin compaction, we constructed nucleosome arrays that are built with a tandem repeat of high affinity nucleosome positioning sequences, which contain probes for DNA accessibility and chromatin structure. I will describe our results that use restriction enzyme digestion and fluorescence resonance energy transfer to determine the probability for DNA site exposure within compacted nucleosome arrays and the time scale for changes in chromatin compaction. I will then discuss how these results help explain how proteins gain access to DNA sites buried within chromatin.

Friday, March 9, 2007 8:00AM - 11:00AM — Session X4 DCMP: Quantum Order in Chiral Magnets Colorado Convention Center Korbel 2B-3B
8:00AM X4.00001 Quantum order in chiral magnets: 3D Non-Fermi Liquid Phase and Blue Quantum Fog in MnSi1. CHRISTIAN PFLEIDERER, Physik-Department E21, Technische Universität München, D-85748 Garching, Germany — The discovery of a distinct change from Fermi liquid to non-Fermi liquid resistivity and the observation of partial magnetic order in MnSi under high pressure [1,2] has generated great scientific interest in the properties of itinerant-electron systems with weak chiral spin-orbit interactions. Recent theoretical predictions include the spontaneous formation of a skyrmion phase at the boundary of conventional helical order [3] and the existence of a new type of Goldstone-like excitation, so called helimagnons [4]. New experimental work using sophisticated neutron scattering techniques and bulk properties exploring the question of skyrmion textures and helimagnon excitations, as well as studies of the thermal expansion under pressure using a newly developed ultra-high resolution neutron spin-resonance technique (Larmor diffraction) will be reviewed.

1 work carried out in collaboration with: P. Böni, M. Janoschek, A. Neubauer, T. Keller and B. Roessli

8:36AM X4.00002 Real Space Observation of Helical Spin Order, MASAYA UCHIDA, Frontier Research System, The Institute of Physical and Chemical Research (RIKEN), Saitama, Japan — When a symmetry gets spontaneously broken in a phase transition, topological defects are routinely formed. There are numerous examples of topological defects in condensed matter systems, such as, vortices in superconductors, vortices in superfluid helium, monopoles and strings in liquid crystals, etc. A similar picture would emerge in helimagnets. It is therefore interesting to deepen our understanding of how, what kind of, and why magnetic defects form and how they evolve after formation in helimagnets. In recent years, there have been significant advances in the experiment [1] and in the theories [2] of phases and textures in helimagnets. This will have a significant impact on our understanding of not only the puzzling behavior of the helimagnet MnSi with non-Fermi-liquid transport properties [3], but also phase transitions and phase diagrams in different condensed matter systems.

In this paper, we describe the current status of our experiments. To see the helical spin order and magnetic defects in metal silicides such as (Fe, Co)Si and FeGe in real space, we used Lorentz electron microscopy, combined with the transport of intensity equation (TIE) analysis or holographic interference microscopy. This method has allowed us to find the topological defect similar to atomic dislocations in the crystal lattice. Furthermore, by applying magnetic fields, we directly observed the deformation processes of the helical spin order, accompanied by nucleation, movement, and annihilation of the magnetic defects.


9:12AM X4.00003 Theory of the helical spin crystals, BENEDIKT BINZ, University of California, Berkeley - now at University of Cologne, Germany — Recent experiments in the “partial order” regime at high pressure in MnSi quite intriguingly suggest diffuse spin correlations and slow dynamics in a pure crystalline metal. As a starting point for a theoretical description of this phase, we are investigating the nature of its dominant spin correlations. Particularly, the observed location of maximal neutron scattering intensity around (110) is difficult to explain in terms of fluctuating helical spin-density waves alone. We therefore investigate helical spin crystals. These are magnetic structures obtained by superimposing distinct spin spirals, via a process reminiscent of crystallization. Based on a phenomenological Landau description, we identify which spin crystal structures may be energetically stabilized and study their properties. One of these states, a bcc spin crystal, is compatible with existing data on MnSi from neutron scattering and magnetic field studies. It also shows new and interesting phenomena, such as symmetry stabilized topological textures, missing higher order Bragg reflections and an octupolar order parameter. Possible routes towards “partial order,” which requires the destruction of long-range order by some mechanism, will be briefly discussed.

9:48AM X4.00004 Investigation of the Metallic State in Cubic FeGe beyond its Quantum Phase Transition, HERIBERT WILHELM, Diamond Light Source, Chilton, Didcot, OX11 0DE, Oxfordshire — FeGe and MnSi are prominent examples where the Dzyaloshinskii-Moriya interaction causes a modulation of the ferromagnetic structure as a consequence of the lack of inversion symmetry in the B20 structure (space group P213). In FeGe, helimagnetism sets in through a first order phase transition at TC = 280K with a saturated moment of m = 1μB per Fe atom. The helical modulation has a period of about 700Å and propagates along the spiral propagation vector k || [100]. It alters its direction to k || [111] at T2 ≈ 211 - 245 K without a change in the period. In MnSi, however, the helical order occurs below TC = 29 K. The modulation has a wavelength of 175Å and the ordered moments of about m = 0.14μB per Mn atom are perpendicular to k || [111]. It is well established that the second order phase transition is driven first order for a sufficiently weak magnetic interaction close to the critical pressure, pc = 1.46 GPa. In light of these structural and magnetic similarities between FeGe and MnSi, a volume compression in FeGe could tune its TC to zero temperature with the chance to reveal peculiar electronic ground state properties at the verge of the magnetic order. Indeed, the electrical resistivity measurements, ρ(T), show a suppression of the helical order at pc ≈ 19 GPa. The strong deviations from a Fermi-liquid behavior in a wide pressure range above pc suggest that the suppression of TC decreases with the standard notion of a quantum critical phase transition. Our band-structure calculations predict that disorder due to zero-point motion is strong enough to close the narrow gap expected for compressed FeGe, stabilizing a new magnetic ground state above pc. An anomaly observed at Tc' in the ρ(T) curves recorded above pc might be related to this magnetic phase. The isothermal structural data at low temperature revealed a discontinuous change in the pressure dependence of the shortest Fe-Ge interatomic distance close to the TC(ρ) phase line. The (T, V) phase diagram will be discussed and the connection with MnSi and the semiconducting properties of FeSi will be addressed.

10:24AM X4.00005 Quantum Phase Transitions and Exotic Phases in Metallic Helimagnets1. DIETRICH BELITZ, University of Oregon — I will review some of the current theoretical understanding of the exotic properties of chiral magnets, in particular the metallic helimagnet MnSi. In the ordered phase, a helical Goldstone mode leads to corrections to Fermi-liquid behavior, and to a non-Fermi liquid single-particle relaxation rate [1]. On the phase boundary, a tricritical point pushes the quantum critical point to a non-zero external magnetic field, where the quantum critical behavior has been determined exactly [2]. In the disordered phase, an analogy with chiral liquid crystals suggests a first-order transition from a chiral liquid to a chiral gas as an explanation for neutron scattering data [3]. The observed non-Fermi-liquid transport behavior in the disordered phase [4] remains an open problem.

1 This work was supported by the NSF under grant Nos. DMR-05-29966, and DMR-05-30314.
8:00AM X27.00001 Superconductor-Insulator Transition in Epitaxial Niobium Nanowires

TIMOTHY MCARDLE, KEVIN INDERHEES, PAUL WELANDER, JAMES ECKSTEIN, University of Illinois, Urbana — As the dimensions of a superconducting nanowire are reduced, it undergoes a transition from a superconductor to an insulator. Near Tc, thermally activated phase slips cause this insulating state, and it is believed that in extremely narrow wires quantum phase slips appear and become dominant at low temperature. However, the exact nature of the S-I transition, specifically what parameters control it, is not clear. We report on recent studies of nanowires fabricated using electron beam lithography from single-crystal niobium films grown by ultra-high vacuum molecular beam epitaxy. Since the films are single crystal, the role of disorder is reduced. Our films are 100 angstroms thick, have transition temperatures near 7.2 K, and residual resistance ratios of around 5, typical for ultra-thin single-crystal niobium films. The wires are 10 µm long and range in width from 35 to 200 nm. This work was supported by the DOE BES at the F. Seitz Materials Research Laboratory at the University of Illinois, Urbana.

8:12AM X27.00002 Imaging of Few-electron InAs Quantum Dots in InAs/InP Nanowires1, ERIN E. BOYD, HALVAR J. TRODAHL, Dept of Physics, Harvard Univ, ANIA BLESZYNSKI, Dept of Physics, Yale Univ, MICHAEL STOPA, Div of Eng and App Sci, Harvard Univ, R.M. WESTERVELT, Dept of Physics and Div of Eng and App Sci, Harvard Univ, LINUS E. FROBERG, LARS SAMUELSON, Dept of Solid State Physics, Lund Univ — InAs quantum dots are promising contenders for nanoelectronics, spintronics and quantum information processing. Their large g-factor makes manipulation of electron spins easier at higher temperatures. InAs dots, as small as 10 nm long holding only a few electrons, can be formed by InP barriers in InAs/InP nanowire heterostructures grown using chemical beam epitaxy. Coulomb blockade transport measurements done using metal contacts and a back gate show excellent results [1]. Using a liquid-He cooled scanning probe microscope, we imaged an InAs quantum dot that holds only one-electron, with the conducting tip as a movable gate [2]. Simulations of electron wavefunctions in the dot show the effect of the back gate and the moveable tip. [1] M. Björk et al., Nano Letters 4, 1621 (2004) [2] A. Bleszynski et al., 28th Int. Conf. Physics of Semiconductors, 2006

8:24AM X27.00003 Imaging Few-Electron Double Quantum Dots in InAs/InP Nanowires1, HALVAR J. TRODAHL, ERIN E. BOYD, Dept of Physics, Harvard Univ, ANIA BLESZYNSKI, Dept of Physics, Yale Univ, R. M. WESTERVELT, Dept of Physics and Div of Engineering & Applied Sciences, Harvard Univ, LINUS E. FROBERG, LARS SAMUELSON, Dept of Solid State Physics, Lund Univ — InAs quantum dots formed in InAs/InP nanowire heterostructures are attractive candidates for nanoelectronics, spintronics and quantum information processing. Tunnel-coupled double InAs dots defined by InP barriers can be grown using chemical beam epitaxy; each dot can be small enough to individually address each dot. With use of a liquid-He cooled scanning probe microscope (SPM), the Coulomb blockade conductance of a single InAs quantum dot in an InAs/InP nanowire has been imaged, using the SPM tip as a movable gate [1]. This approach can individually tune the charge on each InAs dot in an InAs/InP nanowire. We plan to use this technique to investigate tunnel-coupled InAs double dots.


8:36AM X27.00004 Elastodynamics of GaN nanowires at microwave frequencies, COLM FLANNERY, Materials Reliability Division, National Institute of Standards and Technology, Boulder, CO, KRISTINE BERTNESS, Optoelectronics Division, National Institute of Standards and Technology, Boulder, CO, SUDOOK KIM, WARD JOHNSON, Materials Reliability Division, National Institute of Standards and Technology, Boulder, CO — Single-crystal III-nitride nanowires have been the subject of extensive research because of their potential usefulness in innovative electronic, optoelectronics, and sensing applications. They have also been recognized as having several characteristics, including a relatively high surface-to-volume ratio, that are attractive for nanomechanical systems (NEMS) applications, such as mass sensing. In this report, we present Brillouin-light-scattering (BLS) measurements and theoretical modeling of thermally excited vibrational modes in free-standing GaN nanowires with hexagonal cross sections (~70 nm to ~200 nm in diameter) grown from a substrate by catalyst-free molecular beam epitaxy to a length of ~8 µm. A series of modes with frequencies between 8 GHz and 15 GHz are seen in the BLS spectra with axial wavelengths between 270 nm and 1600 nm. Modeling of the normal modes was performed under the approximations that are attractive for nanomechanical systems (NEMS) applications, such as mass sensing. In this report, we present Brillouin-light-scattering (BLS) measurements and theoretical modeling of thermally excited vibrational modes in free-standing GaN nanowires with hexagonal cross sections (~70 nm to ~200 nm in diameter) grown from a substrate by catalyst-free molecular beam epitaxy to a length of ~8 µm. A series of modes with frequencies between 8 GHz and 15 GHz are seen in the BLS spectra with axial wavelengths between 270 nm and 1600 nm. Modeling of the normal modes was performed under the approximations that are attractive for nanomechanical systems (NEMS) applications, such as mass sensing. In this report, we present Brillouin-light-scattering (BLS) measurements and theoretical modeling of thermally excited vibrational modes in free-standing GaN nanowires with hexagonal cross sections (~70 nm to ~200 nm in diameter) grown from a substrate by catalyst-free molecular beam epitaxy to a length of ~8 µm. A series of modes with frequencies between 8 GHz and 15 GHz are seen in the BLS spectra with axial wavelengths between 270 nm and 1600 nm. Modeling of the normal modes was performed under the approximations that are attractive for nanomechanical systems (NEMS) applications, such as mass sensing.
9:12AM X27.00007 Nanoscale Thermal Imaging, KAMAL BALOCH, TODD BRINTLINGER, YI QI, University of Maryland College Park, DAVID GOLDBERGER-GORDON, Stanford University, JOHN CUMINGS, University of Maryland College Park — We present real time, in-situ, high resolution thermal imaging of metallic nanowires. The nanowires are grown on the front-side of silicon nitride membranes. Resistive heating along the wires produces thermal gradients which melt/freeze 20-200nm diameter indium islands deposited by thermal evaporation on the back-side of the membrane. These transitions can be imaged using a transmission electron microscope operating in dark-field mode such that contrast corresponds to the phase of an individual island. Global changes in temperature can be used to calibrate the melting point of individual islands and to account for the presence of the ~100nm thick silicon nitride membrane. Thermal modeling confirms the imaged thermal behavior. This technique could be generally employed for thermal imaging of nanowires and nanotubes, wherein the nanoscale systems are imaged in-situ and under electrical bias. Results of local resistive heating in a carbon nanotube device will also be shown.

9:24AM X27.00008 X-ray Radiation Damage Studies of Individual Nanotubes and Nanowires, H.D. MO, C. NELSON, C.-C. KAO, NSLS, BNL, M. SFEIR, A. BOLLINGER, I. BOZOVIC, J. MIJEWICZ, Dept. of Condensed Matter Phys. & Material Sci., BNL, A. STEIN, Instrumentation Division, BNL, W. LIU, P. ZSCHACK, APS, ANL, N. BOZOVIC, Dept. of Mathematics, San Jose State Univ. — The development of techniques for x-ray studies of individual nanomaterials is motivated by the spectroscopic, structural, and dynamic information that x-rays provide. In combination with other probes (e.g., STM), x-ray techniques promise the complete characterization of nanomaterial properties and functionality, which can be used as feedback for the synthesis of useful nanomaterials. The feasibility of x-ray studies of individual nanomaterials is approaching due to ongoing improvements in x-ray focusing optics and synchrotron radiation sources that together lead to increasing flux densities. However, one possible barrier concerns the effects of high intensity x-ray beams on hard nanomaterials, about which little is currently known. Therefore here we report on x-ray damage studies of individual carbon nanotubes and SrRuO3 nanowires. Samples of the two systems were exposed to microfocused x-rays on APS beamline 34-ID for variable amounts of time. Pre-and post-exposure SEM imaging was used to qualitatively study the effects on carbon nanotubes, and real-time monitoring of sample integrity was provided by measuring a current passing through the SrRuO3 nanowires during the exposure. This research is supported by the DOE, under contracts DE-AC02-98CH10886 (BNL) and W-31-109-ENG-38 (ANL).

9:36AM X27.00009 In-situ and ex-situ analysis of terminal lengths and growth rates of vertically aligned carbon nanotubes grown by acetylene and alcohol catalytic chemical vapor deposition, J. JACKSON, ORNL, K. BELAY, Florida A&M Univ., A. PURETZKY, D. GEOHEGAN, H. CHRISTEN, H. CUI, ORNL — Controlled synthesis of carbon nanotubes (CNTs) at a fast growth rate which produced long, vertically aligned, and containing required number of walls, from MWNT to double- and single-walled nanotubes by varying processing parameters has been achieved in a thermal chemical vapor deposition (CVD) process. Both in-situ optical monitoring and ex-situ characterization methods have been used to determine the terminal lengths and growth rates of CNTs for acetylene, methanol and ethanol feedstocks grown on silicon substrates coated with an aluminum underlayer (~10 nm), molybdenum (~0.2 nm), and iron (~1nm). Maximum growth rates of CNTs were 3-8 times and 50-125 times slower for ethanol and methanol, respectively, compared when using an acetylene feedstock. The terminal lengths of CNT arrays were estimated as: from 200 nm to a few mm for acetylene, ~20 mm for methanol, and ~8 mm for methanol. The terminal lengths, growth rates, the number of walls, and quality of the carbon nanotubes for all three feedstocks show similar temperature dependences. This indicates the existence of a common mechanism responsible for the activation and deactivation of catalyst nanoparticles at different growth temperatures, probably related to catalytic activity and/or the oxidation state of the catalyst nanoparticles. The restart of growth was also observed while controlling subsequent methanol and hydrogen gas flows.

9:48AM X27.00010 Electrical Properties of Individual Semiconducting Oxide Nanobelt and Their Applications*, YI CHENG, P. XIONG, Department of Physics and MARTECH, Florida State University, L. FIELDS, J.P. ZHENG, FAMU/FSU College of Engineering, R. YANG, Z.L. WANG, Georgia Institute of Technology — Field-effect transistors (FETs) with multi-terminal electrical contacts were fabricated on individual oxide (SnO2 and ZnO) nanobelts. Simultaneous two-terminal and four-terminal measurements enable direct correlation of the FET characteristics with the nature of the contacts. Nanobelt FETs with Schottky contacts were found to exhibit n-channel, p-channel or ambipolar characteristics transistors depending on the properties of the contacts. In contrast, low-resistance ohmic contacts on the nanobelts lead to high-performance n-channel depletion mode FETs with well-defined linear and saturation regimes, “on/off” ratio as high as 107, at ambient conditions1. The electron concentration and effective carrier mobility of the nanobelts in different gases at various temperatures were determined from FET measurements on the channel-limited devices. Sensitive electrical response of the SnO2 nanobelt FETs to gas flow containing 0.2-2% H2 was observed at room temperature2. The effort to utilize the channel-limited nanobelt FETs for protein detection will also be reported. *Supported by NSF NIRT grant ECS-0210332. [1] Y. Cheng et al, Appl. Phys. Lett. 89, 093114 (2006). [2] L.L. Fields et al, Appl. Phys. Lett. 88, 263102 (2006).

10:00AM X27.00011 Nonequilibrium electromechanical noise in a nanomechanical resonator, PATRICK TRUITT, JARED HERTZBERG, University of Maryland, KEITH SCHWAB, Cornell University — Current carrying electrons passing through a diffusive conductor can undergo elastic collisions with defects or surface boundaries and thus impart momentum to the lattice. At sufficiently low temperatures, where the electron-phonon scattering length is longer than the mean free path, this electromechanical noise can be driven into equilibrium with the conductor’s thermal noise ( Joule heating). The resulting force from elastic collisions on a doubly-clamped beam was predicted by Shytov et al [1]. We will discuss our low temperature measurements of a gold-coated, radio-frequency nanomechanical resonator. We current bias the conducting layer and monitor the position of the resonator with an RF-SET. From mechanical noise thermometry, we then compare the observed electromechanical noise force with the theory. [1] A.V. Shytov, L.S. Levitov, and C.W.J. Beenakker, Phys. Rev. Lett. 88, 228303 (2002)

10:12AM X27.00012 Electrical-transport properties of individual single-crystalline IrO2 nanorods, Y. H. LIN, Institute of Physics, National Chiao Tung University, Taiwan, T. C. LEE, Y. C. SUN, W. B. JIAN, Department of Electro-physics, National Chiao Tung University, Taiwan, H. M. CHANG, Y. S. HUANG, Department of Electronic Engineering, National Taiwan University of Science and Technology, Taiwan, J. J. LIN, Institute of Physics and Department of Electrophysics, National Chiao Tung University, Taiwan — We have studied the electrical-transport properties of individual single-crystalline IrO2 nanorods (NRs) prepared by MOCVD. With the help of e-beam lithography, individual NRs are contacted by Cr/Au submicron electrodes from above. Utilizing different probe configurations, not only the intrinsic properties of the NRs but also the temperature dependence of the contact resistance, Recontact, has been determined down to liquid-helium temperatures. Our measured resistivity behavior of the NRs is in close agreement with the current theoretical understanding of this material. On the other hand, we found that the temperature behavior of the Recontact obeys the law log Recontact ∝ T−1/2 over a wide temperature range from 100 K down to liquid-helium temperatures. This later conduction process is ascribed to the hopping of electrons through nanoscale metal granules accidentally formed at the contact region during the thermal evaporation of the submicron electrodes.
10:24AM X31.00013 Silicon nanoporous pillar array: template for fabricating silicon-based nanocomposites with enhanced physical properties

XIN JIAN LI, XIAO NAN FU, HAI JUN XU, WEI FEN JIANG
Zhengzhou University — A triple hierarchical structure, silicon nanoporous pillar array (Si-NPA), was formed on silicon wafers by a hydrothermal method. The structure of Si-NPA is characterized by the regular array of micron-sized silicon pillars, quasi-identical nanopores densely distributing over each pillar, and silicon nanocrystals composing the walls of the nanopores. Utilizing the excellent structural regularity and high chemical reactivity of Si-NPA, patterned nanocomposites of CdS, carbon nanotubes (CNTs), Au, and Fe$_3$O$_4$/Si-NPA were fabricated. Their elemental compositions, morphologies and microstructures were characterized. Ideal physical properties of I-V curve in CdS/Si-NPA heterojunction, field emission in Si-NPA, CNTs/Si-NPA, Au/Si-NPA, and humidity/gas sensitivity in Fe$_3$O$_4$/Si-NPA were observed and the corresponding mechanisms were analyzed. These results indicate that Si-NPA could be employed as an ideal template to assemble silicon-based functional nanosystems, and might find multiple applications in fabricating novel electronic devices.

1 Project supported by the NSF of China

10:36AM X31.00014 Growth and Characterization of ZnSe Nanowires on Au-catalyzed Ge substrates

TINA LIN, BENJAMIN COOLEY, NITIN SAMARTH, Dept. of Physics, Penn State University, University Park PA 16802 — Semiconductor nanowires derived from ZnSe are of interest for semiconductor spintronics because of the relatively long spin lifetimes in bulk n-ZnSe. The metal-catalyzed growth of ZnSe nanowires has already been demonstrated on a variety of substrates, including GaP and Si.[1,2]. Here we exploit the formation of a low melting point Au-Ge eutectic alloy to initiate the growth of ZnSe nanowires on Au-covered Ge substrates. ZnSe is deposited under ultrahigh vacuum conditions using solid source molecular beam epitaxy. Scanning electron microscopy reveals the formation of dense random arrays of ZnSe nanowires with typical lengths in the range ~1 - 3µm and diameters of ~10 - 30 nm. We report a systematic study of the effects of growth temperature, thickness of the gold layer, and ZnSe deposition thickness on the characteristics of the resulting ZnSe nanowires. We also report characterization of these nanowires using high resolution scanned probe and electron microscopies, as well as low temperature optical spectroscopy.


Supported by NSF and ONR

Friday, March 9, 2007 8:00AM - 11:00AM —
Session X31 DCMP: Synthesis of Nanotubes and Nanowires Colorado Convention Center 401

8:00AM X31.00001 ABSTRACT WITHDRAWN

8:12AM X31.00002 Bismuth Nanowires: Synthesis, Microscopy and Transport Properties

JASON REPPERT, JIAN HE, MALCOLM SKOVE, BRAD EDWARDS, TERRY TRITT, APPARAO RAO, Clemson University — Thermoelectric materials approaching the atomic level possess unique quantum confinement properties that have generated much interest in recent history. Theoretical investigations have suggested that nanowires with diameters <10 nm will possess a ZT >2. Previously, bismuth nanowires have been successfully synthesized by means of electrochemical deposition, liquid-phase pressure injection, and vapor-phase deposition. Here, we report the synthesis of bismuth nanowires via the pulsed laser deposition method (PLD). Using this approach, we have been successful in producing nanowires ranging in diameters of 10 - 20 nm, with the majority ranging 10 – 12 nm, and lengths 200 - 300 nm. The structure of the as-prepared nanowires was characterized using scanning electron microscopy, high-resolution transmission electron microscopy (HRTEM), scanning transmission electron microscopy, x-ray diffraction and electron diffraction. The HRTEM images of the bismuth nanowires show a crystalline Bi core that is wrapped in an amorphous oxide layer. The lattice spacing of planes parallel to the length of the Bi core was found to be 0.328 nm, corresponding to the (012) planes of Bi. Temperature dependent thermopower measurements obtained from our narrow diameter Bi nanowires will be presented.

8:24AM X31.00003 Growth of Carbon Nanotubes on Metallic Superalloys

SAIKAT TALAPATRA, Southern Illinois University. SWASTIK KAR, SUNIL PAL, PETHURAJA GOPAL, LIJIE CI, ROBERT VAJTAI, PULICKEL AJAYAN, Rensselaer Polytechnic Institute — There are several advantages of growing carbon nanotubes (CNT) directly on bulk metallic substrates, for example in the formation of robust CNT-metal contacts during growth. Recently, we have shown that multi-wall carbon nanotubes can be grown on Inconel 600, a super alloy, using vapor phase catalyst delivery. The single-step growth of high-quality aligned nanotubes (capable to those grown on SiO$_2$ substrates) show encouraging electrical and mechanical properties. This in situ growth opens up a large number of possibilities for nanotube-based devices. Here, we present detailed investigations on the kinetics of the growth under various experimental conditions, and analyze the nanotube growth mechanism on the generic super alloy systems in the framework of our investigations.

8:36AM X31.00004 VLS growth of <111> oriented Silicon nanowires on Si (111) and Si (100); Growth rate dependence of growth defects

JOONHO BAE, Physics Department, University of Texas at Austin, SHAWN COFFEE, JOHN EKERDT, Department of Chemical Engineering, University of Texas at Austin, CHIH KANG SHIH, Physics Department, University of Texas at Austin — Recently, models have been developed to explain the relation between the growth direction and the diameter of VLS grown silicon nanowires. In this study, we present experimental evidences showing growth rate dependence of growth defects such as bending and kink formation of silicon nanowires grown by SiCl$_4$ as a precursor and H$_2$ as a carrier gas. We find that the high growth rate tends to result in nanowires with less growth defects permitting well oriented nanowires. By applying this finding and controlling growth conditions, large area silicon nanowires along <111> direction were successfully demonstrated on Si (111) and Si (100) substrates. On Si (111) substrates, we achieve large area vertically aligned [111] oriented nanowires. On Si (100) substrates, nanowires with four different <111> orientations form a large area of inter-lacing network pattern. The underlying growth mechanism and pattern formation are discussed.

8:48AM X31.00005 Self-assembled Silicon Nanotubes: new 1D semiconductors

MING XIE, JIESHENG WANG, YOKE KHIN YAP, Michigan Tech University — Silicon nanotubes (SiNTs) have recently attracted attention because of the peculiar properties. SiNTs is also compatible to the present Si microelectronic technology. Theoretically, many research groups have investigated the possible existence of SiNTs. Experimentally, amorphous SiNTs have been synthesized by using template methods. Nevertheless, these SiNTs cannot form good crystal structure due to disordered aggregation of silicon atoms in the inner wall of the templates. Recently, self-assembled silicon nanotubes were reported, which have good crystal structure under supercritically hydrothermal conditions. Here we report self-assembled SiNTs via dual RF-plasma treatments. This technique is compatible to the present integrated circuit technology without involving excessive synthesis pressures and temperatures. Furthermore, our SiNTs are vertically aligned on substrates, which can be easily extracted for devices fabrication. Tunneling spectroscopy was used to characterize the local density of states of these SiNTs. Results indicate that these SiNTs are p-type semiconductors, a new 1D semiconductor for future nanoelectronic devices.

1 Corresponding author
Self-Assembly showing no performance deterioration as a result of the placement process. This technique allows for hundreds of working devices to be fabricated with high yield. The electrical properties of the subsequent devices are excellent, is shown to be fully reversible. Once the nanotubes are assembled into the trenches, the molecules are then removed leaving the unfunctionalized SWCNTs.

Beam lithography is then employed to pattern hafnium oxide trenches into which the functionalized SWCNTs selectively bind. The surface functionalization fabrication of large arrays of SWCNT devices. SWCNTs are first functionalized with organic compounds that selectively bind to metal oxide surfaces. Electron placement. This work will highlight recent progress in the selective placement of SWCNTs into predefined positions on gate oxide surfaces, allowing for the Success in the large-scale integration of SWCNTs will depend upon progress in processing to address challenges such as separation, chemical doping and selective placement. This work will highlight recent progress in the selective placement of SWCNTs into predefined positions on gate oxide surfaces, allowing for the fabricated large arrays of SWCNT devices. SWCNTs are first functionalized with organic compounds that selectively bind to metal oxide surfaces. Electron beam lithography is then employed to pattern hafnium oxide trenches into which the functionalized SWCNTs selectively bind. The surface functionalization is especially important that the NW surface be protected against oxidation to avoid uncontrolled property changes. For Ge NWs such oxidation protection is not provided by a stable native oxide (as is the case for Si). Hence, any Ge NW-based devices will require the development of passivation or encapsulation techniques. Here we discuss real-time observations by high-resolution transmission electron microscopy during annealing of individual carbon-supported Ge NWs [1]. At moderate temperatures (~300°C) even thick oxide layers on the Ge NWs are reduced rapidly. This is followed by the assembly of crystalline carbon shells that depends critically on traces of Au on the NW surface originating from the Au/Ge catalyst nanoparticles used for the NW synthesis. We demonstrate that the C-shells provide efficient protection of the Ge NW surface against oxidation in ambient air. More generally, our results point at using metal surface decoration to trigger the encapsulation of a wide variety of NW materials in protective C-shells.

1 Corresponding author
10:36AM X31.00014 Template-Grown TiO2 Single-Nanowires for Gas Sensing. YAPING DAN, University of Pennsylvania, STEPHANE EVOY, University of Alberta, A. T. CHARLIE JOHNSON, University of Pennsylvania — A number of contemporary research efforts are directed towards realization of an “electronic nose” system where a sensor array is coupled to signal-conditioning electronics and sensor responses fed to odor recognition algorithms to perform detection and classification of vapors. Metal oxides thin films and nanowires are candidates for use in such systems, with the latter having performance advantages associated with their small footprint and enhanced quasi one-dimensional carrier confinement. Here we report experiments exploring the use of template-grown TiO2 single-nanowires for gas sensing. TiO2 nanowires were prepared by electroplating Ti(OH)4 sol-gel into anodic aluminum oxide membranes and then annealing at 450 °C for 12 h. These nanowires are typically 10±1μm long and 100±20nm in diameter. When the temperature is elevated from 20 °C to 200 °C, the conductance of a single nanowire increases from 30pS to 330pS, from which an activation energy of 0.51 ± 0.02 eV is extracted. When exposed to 20% O2 at a working temperature of 200 °C, the conductance of the wires increases by 100% within a few seconds. We will report on sensing experiments for O2, H2 and CO with different concentrations as well as the effects of sample annealing and working temperature. This work was supported by the National Science Foundation NIRT Grant #0303961.

10:48AM X31.00015 Self assembly of organic nanostructures and dielectrophoretic assembly of inorganic nanowires. GEETHA DHOLAKIA1, NASA Ames Research Center, STEVEN KUO, NASA Ames, San Jose State University, E. L. ALLEN2, San Jose State University, NASA AMES TEAM, SAN JOSE STATE UNIVERSITY TEAM — Self assembly techniques enable the organization of organic molecules into nanostructures. Currently engineering strategies for efficient assembly and routine integration of inorganic nanoscale objects into functional devices is very limited. AC Dielectrophoresis is an efficient technique to manipulate inorganic nanomaterials into higher dimensional structures. We used an alumina template based sol-gel synthesis method for the growth of various metal oxide nanowires with typical diameters of 100-150 nm, ranging in length from 3-10 μm. Here we report the dielectrophoretic assembly of TiO2 nanowires, an important material for photocatalysis and photovoltaics, onto interdigitated devices. Self assembly in organic nanostructures and its dependence on structure and stereochemistry of the molecule and dielectrophoretic field dependence in the assembly of inorganic nanowires will be compared and contrasted. Tunneling spectroscopy and DOS of these nanoscale systems will also be discussed.

1Center for Aerospace Materials & Devices
2Chemical and Materials Engineering
8:48AM X43.00005 Transient current in a quantum dot asymmetrically coupled to metallic leads. ALI GOKER, PETER NORDLANDER. Department of Physics and Rice Quantum Institute, Rice University, Houston, TX 77251, USA — We use the time-dependent non-crossing approximation to study the transient current for a single electron transistor attached asymmetrically to two metallic leads. We investigate the effects of the bandwidth of the leads, the effect of dot energy level position, the effect of asymmetry in the couplings, and the effects of temperature. In the short timescale, the current reaches a maximum before it starts decaying. In the long timescale, we observe sinusoidal modulations of the current. The frequency of these oscillations is linearly proportional to the bandwidth of the conduction electrons in the leads. The amplitude of these oscillations is found to increase as the temperature is reduced and saturate for temperatures below the Kondo temperature. We discuss the microscopic nature of these oscillations and comment on the possibilities for their experimental detection.

9:00AM X43.00006 Positive correlation in multi-level transport through a tunable quantum dot. YIMING ZHANG, LEONARDO DICARLO, DOUGLAS MCCLURE, Harvard University, MICHISHIYI YAMAMOTO, University of Tokyo and SORST-JST, SEIGO TARUCHA, University of Tokyo and ICORP-JST, CHARLES MARCUS, Harvard University, MICAH HANSON, ART GOSSARD, University of California, Santa Barbara — We report measurements of shot noise auto- and cross-correlation in a tunable quantum dot with two or three leads. As the Coulomb blockade is lifted at finite source-drain bias, the current noise evolves from super-Poissonian to sub-Poissonian in the two-lead case, and the cross-correlation evolves from positive to negative in the three-lead case. The observed super-Poissonian noise and positive cross-correlation are shown to be consistent with transport through excited states.

9:12AM X43.00007 Electron Localization in Strongly Correlated Quantum Dots. A. D. GÜCLÜ, Duke, AMIT GHOsal, UCLA, C. J. UMIRIGAR, Cornell, HAROLD U. BARANGER, Duke — We investigate the electronic properties of quantum dots in the low density regime up to $r_s \sim 60$ using variational and diffusion quantum Monte Carlo methods. Quantum dots are highly tunable systems that allow the study of the physics of strongly correlated electrons. With decreasing electronic density, interactions become stronger and electrons are expected to localize at their classical positions, as in Wigner crystallization in an infinite two-dimensional system. We have studied several multi-determinantal wave functions each built from single-particle states of very different nature – LDA, Hartree, or floating Gaussian orbitals – all optimized using an energy minimization technique. We study the density, pair-density, power spectrum, and addition energy as a function of increasing interaction strength. The main physical picture that emerges is: The system (i) first experiences a competition between different possible classical configurations, namely either the magic angular momentum states of the shell structure or those of the quantum mechanical symmetry, and (ii) then finally reaches the strongly localized regime consistent with the classical ground state.

9:24AM X43.00008 Magnetic-field evolution of collective excitations in InGaAs/GaAs few-electron quantum dots in the mK regime. SOKRATIS KALLIAKOS, CESAR PASCUAL GARCIA, VITTORIO PELLEGRI, NEST CNR-INFN and Scuola Normale Superiore, Pisa, Italy, AIRON PINCZUK, Dept of Physics, Dept of Appl. Phys. and Appl. Math., Columbia University, New York, New York, BRIAN S. DENNIS, LOREN N. PFEIFFER, KEN W. WEST, Bell Labs, Lucent Technologies, Murray Hill, New Jersey, MASSIMO RONTANI, GUIDO GOLONI, ELISA MOLINARI, S3 CNR-INFN and Università degli Studi di Modena and Reggio Emilia, Modena, Italy — Spin transitions and interactions in few-electron quantum dots (QDs) are investigated by resonant inelastic light scattering (ILS). Here we present the observation of inter-shell excitations in GaAs/AlGaAs QDs that are fabricated by combining e-beam nano-lithography with high quality reactive ion etching. The interpretation of the experimental results by numerical evaluations within a full configuration interaction approach highlights the importance of the exchange and correlation effects in these systems. We show that, under the impact of a perpendicular magnetic field, the evolution of electronic spin and charge inter-shell excitations at mK temperatures reveal that significant changes in the ground state occur even at moderate magnetic fields. These experiments demonstrate that ILS enables the study of few-electron effects in QDs under the extreme conditions of low temperatures and high magnetic fields.

9:36AM X43.00009 ABSTRACT WITHDRAWN —

9:48AM X43.00010 ABSTRACT WITHDRAWN —

10:00AM X43.00011 Electronic Structure of PbSe/PbS Core-Shell Quantum Dots. ADAM BARTNIK, Cornell University, EFRAT LIFSHITZ, Israel Institute of Technology, FRANK WISE, Cornell University — The electronic structure of PbSe/PbS core-shell Quantum Dots (QDs) is calculated within a 4-band envelope function theory and compared to experimentally observed absorption spectra [1]. Our theory extends the isotropic effective mass approximation used successfully in PbS and PbSe core QDs [2] to be valid across discontinuous barriers in material parameters. Even though the band gaps of PbSe and PbS present a Type-II heterostructure, the model predicts that at typical QD sizes, these Type-II effects will not be seen. In fact, the wavefunctions are predicted to extend evenly over both materials except in the largest of sizes. This unusual lack of confinement is explained, and is shown to agree well with recent experimental results. [1] E. Lifshitz, et. al. Air-stable PbSe/PbS and PbSe/PbSe quantum dots and their applications. Journal of Physical Chemistry B, 2006. [2] I. Kang and F. W. Wise. Electronic structure and optical properties of PbS and PbSe quantum dots. J. Opt. Soc. Am. B, 14(7):1632, July 1997.

10:12AM X43.00012 Investigation of Individual InGaAs Quantum Dots by Cross-Sectional Ballistic Electron Emission Microscopy (BEEM). S.Y. LEHMAN, The College of Wooster, J.P. PEHZ, C. MARGINEAN, The Ohio State University, J.G. CEDERBERG, Sandia National Laboratories — Quantum dots (QDs) in III-V semiconductors are of great technological interest, but electronic properties of individual QDs are difficult to measure. We are using cross-sectional BEEM for this purpose. Multiple layers of InAs and In$_{0.4}$Ga$_{0.6}$As QDs were grown by organometallic phase epitaxy, with the thickness of deposited material ranging from subcritical to that generating $5 \times 10^{10}$ dots/cm$^2$. The QD layers were separated by n-doped ($5 \times 10^{16}$ cm$^{-3}$) GaAs/Al$_{0.3}$Ga$_{0.7}$As layers of combined thickness ranging from 130 to 190 nm. The sample was cleaved ex situ and 5nm-thick Au Schottky barrier (SB) contacts were deposited on the cleaved edge using a shadow mask [1]. UVH BEEM at 300 K was used to locate and image the QDs and adjacent layers. The local conduction band energy (as measured by the SB height) ranged from ~0.7 eV at cleaved or near-surface QDs up to ~1 eV over the AlGaAs layers. Surprisingly, the BEEM current amplitude over particular QD layers appears to vary non-monotonically with In content. On-going work will be discussed to use low temperature BEEM with an applied reverse bias to measure the energy depth and physical depth of the cleaved QDs. Work supported by NSF Grant No. DMR-0505165. [1] C. Tivarus et al., PRL 94, 206803 (2005).

10:24AM X43.00013 ABSTRACT WITHDRAWN —
10:36AM X43.00014 Composite fermion solid and liquid states in two component quantum dots 
CHUNTAI SHI, Department of Physics, 104 Davey Laboratory, The Pennsylvania State University, Pennsylvania, 16802, GUN SANG JEON, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, JAINENDRA K. JAIN, Department of Physics, 104 Davey Laboratory, The Pennsylvania State University, Pennsylvania, 16802 — We consider correlated states of a quantum dot, at high magnetic fields, assuming electrons with two components. This model has possible relevance to quantum dots in a bilayer system, a two valley system, in graphene, or for ordinary GaAs based quantum dots in the limit of small Zeeman energy. We show that both the liquid states and crystallites (the latter occurring at large angular momenta) are accurately described in terms of composite fermions. The residual interaction between composite fermions is important, however, and causes complex nearest and next-nearest neighbor spin correlations in the composite fermion crystallite.

10:48AM X43.00015 Dephasing of an electron Mach-Zehnder interferometer capacitively coupled to a quantum dot. SEOK-CHAN YOUN, HEUNG-SUN SIM, Korea Advanced Institute of Science and Technology, HYUN-WOO LEE, Pohang University of Science and Technology — We theoretically investigate an electron Mach-Zehnder interferometer capacitively coupled to a quantum dot. We derive the current and connect its interference behavior to the statistics of the charge fluctuation of the dot. The interference is analyzed in the two limiting cases of fast and slow charge fluctuations: For the case of fast fluctuations where the dwell time of the dot is much smaller than the flight time of the interferometer, the visibility is reduced due to the charge fluctuations, while in the opposite limit the behavior of the interference can be understood by screening effects. The connection to recent experimental and theoretical works will be discussed.

Friday, March 9, 2007 11:15AM - 2:15PM —
Session Y1 DCMP: Fractional Quantum Hall Effect: Spin Effects and Broken-translational-symmetry States Colorado Convention Center Four Seasons 2-3

11:15AM Y1.00001 Low frequency spin dynamics in a quantum Hall canted antiferromagnet,
KOJI MURAKI, NTT Basic Research Laboratories — In quantum Hall (QH) systems, Coulomb interactions combined with the macroscopic degeneracy of Landau levels (LLs) drive the electron system into strongly correlated phases as illustrated by the series of fractional QH effects and may also lead to various forms of broken symmetry dictated by the LL filling factor ν. When two layers of such electron systems are closely separated by a thin tunnel barrier, the addition of interlayer interactions and the layer degree of freedom brings about even richer electronic phases, opening up possibilities for different classes of symmetry breaking. In particular, at total filling factor ν∗ = 2, where the two of the four lowest LLs split by the Zeeman and interlayer tunnel couplings are occupied, the competing degrees of freedom due to the layer and spin are predicted to lead to rich magnetic phases. Here we present results of resistively detected nuclear spin relaxation measurements in closely separated electronic systems that reveal strong low-frequency spin fluctuations in the QH regime at ν∗ = 2 [1]. As the temperature is decreased, the spin fluctuations, manifested by a sharp enhancement of the nuclear spin-lattice relaxation rate 1/T1, continue to grow down to the lowest temperature of 66 mK. The observed divergent behavior of 1/T1 signals a gapless spin excitation mode (i.e., a Goldstone mode) and is a hallmark of the theoretically predicted canted antiferromagnetic order. Our data demonstrate the realization of a two-dimensional system with broken planar spin rotational symmetry, in which fluctuations do not freeze out even at approaching the zero temperature limit. [1] N. Kumada, K. Muraki, and Y. Hirayama, Science 313, 329 (2006).

11:51AM Y1.00002 Density dependent anisotropic phases in a two-dimensional hole system.
MICHAEL MANFRA, Bell Laboratories — Anisotropic charge transport is observed in a two-dimensional (2D) hole system in a perpendicular magnetic field at filling factors ν=7/2, ν=11/2, and ν=13/2 at low temperature. In stark contrast, the transport at ν=9/2 is isotropic for all temperatures. Our results for a 2D hole system differ substantially from 2D electron transport where no anisotropy has been observed at ν=7/2, and the strongest anisotropy occurs at ν=9/2. Isotropic hole transport at ν=13/2, 11/2 and 7/2 is restored for sufficiently low 2D densities. The density dependence of the observed anisotropies suggests that strong spin-orbit coupling in the hole system contributes to the unusual transport behavior.

12:27PM Y1.00003 Spectroscopy of quasiparticle excitations in quantum Hall fluids.
ARON PINCZUK, Columbia University — Quantum Hall fluids support low-energy excitation modes that are linked to remarkable behaviors that emerge from fundamental interactions in two-dimensions. Inelastic light scattering methods at very low temperatures (below 1 Kelvin) offer unique experimental venues to study excitations in the charge and spin degrees of freedom of the fluids. This talk presents an overview of recent results. The focus is on low-lying excitations that express distinct quantum phases of the electron liquids. The experiments offer insights on translational symmetry, on magnetoroton excitations and on quasiparticle energy level structure. The excitations are probed in diverse states of the electron liquids to provide insights on quasiparticle properties and on the phase transformations between quantum fluid states.

In collaboration with Y. Gallais, J. Groshaus, J. Yan, T. Kirschenmann, C.F. Hirjibehedin, I. Dujovne, B.S. Dennis, L.N. Pfeiffer and K.W. West.

1:03PM Y1.00004 Microwave Spectroscopy of Wigner crystals in 2DES and Bilayer systems:
Many-body correlation in electronic quantum solids.
YONG P. CHEN, Rice University — It is generally known that in high quality two dimensional electron systems (2DES, similarly for 2D hole systems and bilayer systems) under sufficiently large perpendicular magnetic field B, the quantum Hall (QH) states terminate into an electronic solid — a Wigner crystal (WC) pinned by disorder. After a brief review of solid phases in QH systems (including several recently discovered ones [1]) as known from microwave spectroscopy (measuring a characteristic pinning mode resonance of the solid), I will show two of our experiments that highlight the importance of many-body quantum correlation in the high-B WC. In one experiment [2], we measured the melting temperature (Tc) of the high-B WC at many different B and densities n and in multiple 2DES samples. The data show unambiguously that in a given sample, Tc is controlled by Landau filling v=nh/eB instead of by n. This demonstrates the quantum nature of the high-B WC and that its melting is dependent only on many-body quantum correlation (via v). Such behavior contrasts with any other known solids (in particular, a classical electron solid), whose Tc are determined by n. In addition, we found that stronger pinning disorder in samples with tighter vertical confinement led to an enhancement of Tc. In another experiment [3], we studied bilayer WC (BWC) in bilayer hole systems (in low inter-layer tunneling limit). We found that in samples with a bilayer exciton condensate (BEC) QH state at v=1, the pinning mode frequency of the BWC (ν=1) is systematically enhanced from what would be expected from two classically interacting single-layer WC. The enhancement decreases with increasing effective layer separation and is not observed for samples without the ν=1 state. We suggest that our results give evidence for pseudospin (layer index) ferromagnetic BWC, which possesses interlayer quantum correlation and long range in-plane phase coherence similar to that in the ν=1 BEC state and can experience enhanced pinning [4] in the presence of interlayer spatial correlation of disorder. [1] Yong P. Chen et al., Phys. Rev. Lett. 93, 206805 (2004); Phys. Rev. Lett. 91, 016801 (2003); [2] Yong P. Chen et al., Nature Physics 2, 452 (2006); [3] Z. Wang et al, submitted; [4] Yong P. Chen, Phys. Rev. B 73, 115314 (2006).

1Work done at Princeton University and National High Magnetic Field Laboratory.
1:39PM Y1.00005 Interweaving of Spin and Pseudospin in Bilayer Quantum Hall Systems¹, H.A. FERTIG, Indiana University, Bloomington, IN and Technion, Haifa, Israel — In a bilayer quantum Hall system, the layer index may effectively act like a two-valued degree freedom that is analogous to the spin of the electron. Near filling factor \( \nu = 1 \) this pseudospin is thought to lock into a linear combination of the two possible values of the layer index, yielding an interlayer coherent state analogous to an easy-plane ferromagnet. Such systems possess excitations known as merons, vortex-like objects in which the pseudospin tilts out of the plane near their cores. In quantum Hall systems these are charged objects, and can be injected into the groundstate by doping away from \( \nu = 1 \), yielding a pseudospin textured state. However, recent experiments [1] have suggested that charged excitations may tilt the real electron spin away from its most polarized state. In this work [2] we study the possibility of simultaneously producing both spin and pseudospin textures in a quantum Hall bilayer near \( \nu = 1 \). Our Hartree-Fock calculations demonstrate that the groundstate generically forms a textured crystal, and that for appropriate choices of Zeeman coupling, interlayer tunneling, interlayer separation, and interlayer bias, the texture can be present in both the spin and pseudospin degrees of freedom. Such states spontaneously break the real rotational spin symmetry and possess a gapless spin wave mode. The possible relevance of this to understanding DMR relaxation rates observed recently in experiment is discussed.

¹This work was performed in collaboration with J. Bourassa, B. Roostaei, R. Cote, and K. Mullen, and was supported by NSF.

Friday, March 9, 2007 11:15AM - 1:39PM –

Session Y3 DCMP: Exotic electronic structures of complex materials and phases Colorado Convention Center Korbel 2A-3A

11:15AM Y3.00001 The electronic structure of a liquid Pb film. JÜRGEN OSTERWALDER, Physics Department, University of Zurich, Switzerland — Our understanding of the electronic structure of condensed matter in the liquid phase is far from complete. We used angle-resolved photoemission spectroscopy (ARPES) in order to study the evolution of the electronic bands, the Fermi surface and the spectral function of a lead monolayer on Cu(111) as the film went through its melting transition at 568 K [1]. The crystalline copper substrate provides the reciprocal lattice vectors, absent in the liquid state, that are needed in ARPES for wave-number conservation in the excitation process, and the well-resolved copper bands serve as an important reference frame for identifying the dramatic changes in the lead states. Electron spectra and momentum distribution maps of the liquid film reveal three important features: the persistence of a Fermi surface, the filling of band gaps, and the localization of the wave functions upon melting. Distinct coherence lengths for different sheets of the Fermi surface are found, indicating a strong dependence of the localization lengths on the character of the constituent atomic wave functions.


11:51AM Y3.00002 Thin-Film Electronic Structure: Beyond the “Particle in a Box” Model, T. MILLER, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign — The quantization of electronic states in thin metallic films is now well-established, having been observed in a number of systems including films on metal as well as semiconductor substrates. The impact of this quantization on the films’ physical properties has been demonstrated in several studies, including the dependence on thickness of films’ thermal stabilities, work functions, and superconductivity transition temperatures. In the simplest model, the electrons are confined to the film by the substrate and vacuum interfaces, which work as “mirrors” to reflect the electrons back into the film, resulting in discrete standing-wave states. In this picture, the substrate forms a reflecting barrier due to a mismatch of electronic structures between it and the overlayer, and the main result is the formation of discrete energy subbands. In this talk, photoemission results will be presented from a variety of thin-film systems that show more interesting electronic structures due to interactions with the substrate and interface. The systems studied highlight different effects, including interfacial scattering and diffraction, hybridization of film and substrate states, and the formation of a composite quantum well from a thin metallic film on a semiconductor. In the latter case, the semiconductor depletion region forms part of the system via coherent coupling between film and substrate electronic states. In collaboration with S. J. Tang, N. J. Speer, D. Ricci, M. Upton, L. Basile, S.-L. Chang, Y.-R. Lee, and T.-C. Chiang.

12:27PM Y3.00003 Ultrahigh-resolution photoemission from superconductors and strongly-correlated materials, SHIK SHIN, University of Toyko — I would like to introduce the ultra-high resolution photoemission study of several superconductors and strongly correlated materials using UV-laser-photoemission [1]. The laser-PES system has the performance of about 360-eV energy resolution, and pseudospin textures in a quantum Hall bilayer near \( \nu = 1 \). Our Hartree-Fock calculations demonstrate that the groundstate generically forms a textured crystal, and that for appropriate choices of Zeeman coupling, interlayer tunneling, interlayer separation, and interlayer bias, the texture can be present in both the spin and pseudospin degrees of freedom. Such states spontaneously break the real rotational spin symmetry and possess a gapless spin wave mode. The possible relevance of this to understanding DMR relaxation rates observed recently in experiment is discussed.

¹This work was performed in collaboration with A. Bostwick, T. Ohta, J. L. McChesney (LBNL), Th. Seyller (U. Erlangen), K. Horn (Fritz Haber Institute).

1:03PM Y3.00004 The spectral function and quasiparticle dynamics of graphene thin films, ELLI ROTENBERG, Lawrence Berkeley National Laboratory — Graphene, a single layer of carbon atoms arranged in a simple honeycomb lattice, is the building block of graphite, fullerenes, and carbon nanotubes and has fascinating electronic properties deriving from the effectively massless, relativistic behavior of its crystal, and that for appropriate choices of Zeeman coupling, interlayer tunneling, interlayer separation, and interlayer bias, the texture can be present in both the spin and pseudospin degrees of freedom. Such states spontaneously break the real rotational spin symmetry and possess a gapless spin wave mode. The possible relevance of this to understanding DMR relaxation rates observed recently in experiment is discussed.

³Work done in collaboration with A. Bostwick, T. Ohta, J. L. McChesney (LBNL), Th. Seyller (U. Erlangen), K. Horn (Fritz Haber Institute).

Friday, March 9, 2007 11:15AM - 1:39PM –

Session Y5 GSNP DCMP: Fluctuating Random Solids and their universal properties Colorado Convention Center Korbel 1A-1B

11:15AM Y5.00001 Nonaffine deformations in random solid media, BRIAN DIDONNA, University of California, Los Angeles — The elastic properties of materials which are inhomogeneous on mesoscopic length scales is a subject of broad interest in soft matter physics. Example systems include stiff polymer or biopolymer gels, foams, emulsions, grain packs, and microstructured solids. These diverse systems share the common feature that their linear elastic response is highly non-uniform, or “non-affine” at intermediate length-scales. I will present a general theoretical framework for interpreting the non-affine component of the linear elastic response of inhomogeneous materials. I will outline the connection between measured correlation functions and internal quantities such as correlation length and internal stress fields, and the dynamics of local elastic heterogeneity. I will show that the simplest 2-point correlation function gives misleading results in 2 dimensions, and I will propose better functions to measure.

11:51AM Y5.00002 Identifying Collective Modes in d_{x^2−y^2}-wave Superconductors via Impurities, ROY NYBERG, DIRK MORR, ENRICO ROSSI, University of Illinois-Chicago — We demonstrate that magnetic impurities can be employed to identify the behavior of a disordered network of conductors near its percolation point. Due to the presence of strong correlations, “checkerboard” patterns are dispersionless. Additionally, by using variational Monte Carlo method, we show that the impurity scattering are greatly suppressed by interference. We are able to obtain all these features seen by STM experiments in both real- and momentum- space. Our results also show that the observed state (LDOS) on the surface of high-Tc superconductors support the idea that remains finite for all p > p_c and which vanishes with a characteristic power law G(p, T) ~ (p − p_c)^{θ}. Our simulations in both two and three dimensions seem to indicate that T is model-independent and, within our error bars, the same as the exponent that describes the behavior of a disordered network of conductors near its percolation point.

12:27PM Y5.00003 Floppy modes and non-affine deformations in biopolymer networks, ERWIN FREY, Ludwig-Maximilians-Universitaet Muenchen — Fibrous materials are ubiquitous in nature. They form the cytoskeleton of cells and are essential components of the extracellular matrix. Its building blocks are stiff protein filaments and a myriad of associated crosslinking proteins. The interplay between the elasticity of the biopolymers and the binding and elastic properties of the crosslinkers lead to a variety of network architectures [1]. We review recent advances in understanding the elastic properties of these networks in terms of “floppy modes” [2], which are the relevant low-energy excitations characterizing non-affine deformations. This approach might very well serve as a novel paradigm to understand the elasticity of microstructured materials. The theoretical concepts are applied to recent experimental studies of F-actin networks crosslinked with fascin. [1] C. Heussinger and E. Frey, Stiff Polymers, Foams and Fiber Networks, Phys. Rev. Lett. 96, 017802 (2006). [2] C. Heussinger and E. Frey, Floppy Modes and Non-Affine Deformations in Random Fiber Networks, Phys. Rev. Lett. 97, 105501 (2006)

1:03PM Y5.00004 Molecular dynamics studies of rigidity in solids, MICHAEL PLISCHKE, Simon Fraser University — We have used molecular dynamics (MD) to study the elastic properties of systems of particles randomly and permanently crosslinked to each other as function of crosslink density p. At zero temperature, such systems generically lose the ability to withstand shear at a rigidity percolation point, p_r, that is (at least for particles interacting through central forces) different from the geometric percolation point p_c. At finite temperatures there is an entropy-generated component of the shear modulus G(p, T) that remains finite for all p > p_c and which vanishes with a characteristic power law G(p, T) ~ (p − p_c)νT. Our simulations in both two and three dimensions seem to indicate that T is model-independent and, within our error bars, the same as the exponent that describes the behavior of a disordered network of conductors near its percolation point.

Friday, March 9, 2007 11:15AM - 1:39PM –
Session Y8 DCMP: Superconductivity: Theory Colorado Convention Center Korbel 1C

11:15AM Y8.00001 Impurity scattering interference in high-Tc superconductors, CHUNG-PIN CHOU, TING KUAO LEE, NOBORU FUKUSHIMA, Academia Sinica — Recent STM measurements have observed many inhomogeneous patterns of the local density of state (LDOS) on the surface of high-Tc cuprates. In particular, for Bi2212 crystals, well defined interference patterns in the momentum space have been seen at low bias voltage. And recently, for the underdoped sample, it has been observed that the spatially “checkerboard” LDOS modulations appear at higher energies. By using a simple impurity scattering potential with BCS Hamiltonian, we describe all LDOS features in Bi2212 materials in terms of quasiparticle scattering on the energy scale of the superconducting gap without inducing an impurity states inside the gap. Moreover, the spin-resolved LDOS exhibits characteristic differences on the two sublattices of the antiferromagnetic droplet. This effect, together with the spatial dependence of the LDOS provides inside into the characteristic momentum of the mode as well as its correlation length. Since these features are absent for other collective modes such as phonons or charge-density waves, our study provides future experiments with the possibility to identify the nature of collective modes.

11:27AM Y8.00002 Identifying Collective Modes in d_{x^2−y^2}-wave Superconductors via Impurities , ROY NYBERG, DIRK MORR, ENRICO ROSSI, University of Illinois-Chicago — We demonstrate that magnetic impurities can be employed to identify the nature of collective modes in the cuprate superconductors. Specifically, we show that a magnetic impurity in an external magnetic field pins an antiferromagnetic collective mode, thus inducing to a local spin-density wave (SDW), i.e., a magnetic droplet. Using a scattering T-matrix formalism, we find that the presence of such a droplet significantly changes the local electronic structure of the d_{x^2−y^2}-wave superconductor. In particular, it suppresses the local density of states (LDOS) inside the droplet on the energy scale of the superconducting gap without inducing an impurity states inside the gap. Moreover, the spin-resolved LDOS exhibits characteristic differences on the two sublattices of the antiferromagnetic droplet. This effect, together with the spatial dependence of the LDOS provides inside into the characteristic momentum of the mode as well as its correlation length. Since these features are absent for other collective modes such as phonons or charge-density waves, our study provides future experiments with the possibility to identify the nature of collective modes.
11:39 AM Y8.00003 Identifying Collective Modes in \( d_{x^2-y^2} \)-wave superconductors via Impurities: II, DIRK MORR, ROY NYBERG, ENRICO ROSSI, University of Illinois at Chicago — In the preceding talk, we demonstrated that magnetic impurities can be employed to identify the nature of collective modes in the cuprate superconductors. In particular we showed that a magnetic impurity in an external magnetic field pins an antiferromagnetic spin mode and induces to a local magnetic droplet. This droplet in turn changes the local electronic structure of the \( d_{x^2-y^2} \)-wave superconductor. Using a non self-consistent \( T \)-matrix formalism, we identified several characteristic features in the local density of states (LDOS) that arise from the presence of the magnetic droplet. The question naturally arises whether the suppression of the superconducting order parameter (SCOP) in the droplet will alter our conclusions. To investigate this question, we employed a Bogoliubov de Gennes formalism that allows us to self-consistently compute the spatial form of the SCOP. Our results are two-fold. First, we find that the SCOP is significantly changed from its bulk value only in the center of the droplet, and that it recovers the bulk value within a few lattice spacings from the center of the droplet. Second, the suppression of the SCOP only leads to small quantitative changes in the LDOS. Hence our conclusions obtained within the \( T \)-matrix formalism remain unchanged.

\footnote{We acknowledge financial support by NSF and DOE}

11:51 AM Y8.00004 Dispersing and non-dispersing peaks and two-energy scales in AC-Arpes in underdoped cuprates, BELEN VALENZUELA, ELENA BASCONES, Instituto de Ciencia de Materiales de Madrid — Recent experiments have shown that the structure in Autocorrelation (AC) Arpes maps compare well with the one observed in Fourier Transform Scanning Tunneling Spectroscopy (FT-STS). In particular dispersing peaks (consistent with the octet model due to scattering induced interference) are observed at low energies in the superconducting state and non-dispersing ones are seen in the pseudogap state and at higher energies in the superconducting state of underdoped cuprates. We have computed the AC-Arpes using the Yang, Rice and Zhang (YRZ) model for the pseudogap. This model assumes that pseudogap and superconductivity compete below a critical doping and has been successfully used (cond-mat/0611154) to explain the two energy scales found in Raman and ARCES experiments below \( T_c \). We will show that the computed AC-ARPES compares well with the experimental results. The pseudogap is characterized by non-dispersing peaks. In underdoped superconducting cuprates with pseudogap scale larger than the superconducting order parameter, dispersing peaks, associated to the non-dispersing order parameter appear at low energies and non-dispersing ones, related to the pseudogap, at higher energies.

12:03 PM Y8.00005 From the BCS equations to the Anisotropic Superconductivity equations. JOSE SAMUEL MILLAN, Universidad Autonoma del Carmen, Luis Antonio Perez, Instituto de Fisica, Universidad Nacional Autonoma de Mexico (UNAM), CHUMIN WANG, Instituto de Investigaciones en Materiales, UNAM — Since the discovery of cuprate superconductors, many new correlated electronic models have been proposed in order to understand their substantially different features, such as high transition temperature \( (T_c) \) at an optimal doping, quasi two-dimensional behavior, d-symmetry superconducting order parameter, less influence of the isotope effect, and a power-law behavior of the superconducting specific heat. Recently, we have studied a two-dimensional generalized Hubbard model, in which a second-neighbor correlated hopping is included in addition to the on-site and nearest-neighbor repulsions [1]. This model has the advantage to be able to give some insights on all these new features within the BCS formalism. In this work, we report a unified description of s-, \( d \)-, and d-wave superconductivities, in which the experimental power-law behavior of anisotropic superconducting specific heat can be nicely reproduced [2]. [1] J. S. Millán, L. A. Pérez, and C. Wang, Phys. Lett. A 335, 505 (2005). [2] J. S. Millán, L. A. Pérez, and C. Wang, Proceedings of AIP 850, 563 (2006).

12:15 PM Y8.00006 ABSTRACT HAS BEEN MOVED TO C1 —

12:27 PM Y8.00007 Tuning effective interactions in high-\( T_c \) cuprates via apical oxygen atoms: New realization from the first-principles Wannier function approach, WEI GUO VIN, WEI KU, Brookhaven National Laboratory — Based on a novel first-principles Wannier function approach, the low-energy effective Hamiltonian for high-\( T_c \) cuprates is derived. The apical oxygen atoms are found to significantly modify the mobility and distribution of the Zhang-Rice singlets in the \( CuO_2 \) plane, by tuning the effective hopping parameters \( t' \) and \( t'' \), and local chemical potential, \( \mu_{\text{eff}} \). Most remarkably, \( V_{\text{eff}} \), an additional effective repulsion (de- pairing) between neighboring doped holes, is found to be significantly tuned by a "vacuum fluctuation" mechanism inherited from the correlated multiband nature of the cuprates. Our results identify the apical oxygen states as the main material dependence of these systems and provide a microscopic avenue to the understanding of recent spectroscopic imaging STM data [K. McElroy et al., Science 309, 1048 (2005)].

12:39 PM Y8.00008 Realistic Model of Cuprate High-Energy Pseudogaps, J.C. PHILLIPS, Rutgers University — Cuprates become metallic only when doped, much like semiconductor impurity bands. The unique properties of the cuprates are the result of self-organization of the dopants to form off-lattice filamentary networks ("pearls on strings"). The internal structure of these glassy networks is optimized by maximizing their dielectric screening of internal ionic fields. At low energies ARPES peaks in energy and momentum distributions give similar quasiparticle dispersions, but at \( \frac{\hbar}{m} \approx 0.5 \) eV, a step-function jump in the relaxation of spectral holes at 1.5 eV; all the Lanzara angular isotopic trends observed across the phase diagram by ARPES, and the two Ando lines in the planar resistivity occurring at the pseudogap transition \( T^* \) and at optimal doping; the Shen Fermi arcs that evolve with doping, whose angular strength ratio has a step-function at optimal doping; a similar step-function jump in the relaxation of spectral holes at 1.5 eV; all the Lanzara angular isotopic trends observed across the phase diagram by ARPES, and the diamagnetic anomalies associated with the pseudogap, with onset temperatures \( T \) as large as \( 2T_{\text{max}} \).

12:51 PM Y8.00009 High-\( T_c \) superconductivity originates in BaO or similar planes, not in cuprate-planes, JOHN D. DOW, Arizona State University — \( CuO_2 \) planes are not needed for high-\( T_c \) superconductivity, as demonstrated by \( Sr_2YRuO_4 \) and \( Ba_2YRuO_6 \), weakly doped on Ru sites with Cu but having no cuprate-planes. These materials have onsets of superconductivity at 49K and 93K, respectively. We have shown that the related Cu-Ru materials \( Gd_{2-x}Ce_xSr_2Ru_2O_{16} \) and \( GdSr_2Cu_2RuO_6 \) do not superconduct in their cuprate planes, which are magnetic, but in their \( Sr \)O layers (with onset \( T \approx 45K \)) [1]. The claims that the cuprate-planes superconduct are based on a one-point unconfirmed jump in the Bell Labs data that was supposedly confirmed by Jorgensen [2], although Jorgensens data actually contradict the Bell datum. In all the materials we have studied, and even in \( YBa_2Cu_3O_7 \), the superconductivity occurs in the bulk in layers that do not contain Cu, namely in \( BaO \) layers of \( YBa_2Cu_3O_7 \), which have s-wave character, not d-wave character [3].

\footnote{CSIC and CAM through grant 200550M136 are acknowledged}


\footnote{J. D. Jorgensen, Phys. Today, 34 (June, 1991).}

\footnote{D. R. Harshman et al., Phys. Rev. B 69, 174505 (2004).}
1:03PM Y8.00010 Ba$_2$YRuO$_6$: High-\(T_c\) superconductivity without CuO$_2$ planes.  HERMANN AZEMTSA DONFACK, Arizona State University — Doped Ba$_2$YRuO$_6$ begins superconducting at 93 K, although it has no cuprate-planes. It does have Cu as a dopant, but superconducting with so little Cu (1%) [S. M. Rao et al., J. Crystal Growth 235, 271 (2002)] that it is clearly not a cuprate-plane superconductor. This means that CuO$_2$ planes are not needed for high-\(T_c\) superconductivity. It also means that all theories of high-\(T_c\) superconductivity based on cuprate-planes superconducting are incorrect, or else that there are at least two theories of high-\(T_c\) superconductivity, not just one: one for cuprate-plane materials, and one for ruthenates. (It is our opinion that there is just one theory of high-\(T_c\) superconductivity.

2:27PM Y8.00012 Superconductivity in the ordered limit1. VLADIMIR CVETKOVIC, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218 — A novel mechanism for superconductivity is proposed based on the duality in the quantum elasticity. Using a charge crystal as a starting point, these superconductors can be viewed as liquid crystal phases of charge in sense that the broken translational symmetries are restored by the Bose condensation of dislocation defects. Although the crystalline correlations are lost at long distance, the order (and the shear rigidity of the solid) persists at scales large enough to be observable. This leads to a host of unconventional properties predicted for this ‘ordered’ superconductor: Meissner effect with oscillating screening, screening of Coulomb force, long-range topological order, and the presence of a new excitation in the dynamical electric response. The origin of this excitation lies in the short-range shear rigidity, i.e., transient order of a solid. Therefore, an experiment designed to measure the presence of the predicted excitations in the cuprate superconductors could be used to unambiguously (dis)prove the existence of fluctuating stripes.

Supported by the Netherlands foundation for fundamental research of Matter (FOM) and in part by the NSF grant DHR-0531159.

Friday, March 9, 2007 11:15AM - 2:15PM
Session Y27 DCMP: Nanowire Sensors and Oscillators Colorado Convention Center 301

11:15AM Y27.00001 Effect of Chamber Pressure on the Vibrational Properties of Micro- and Nano-Cantilevers, GAYATRI KESKAR, JAY GAILLARD, JONATHAN TAYLOR, MALCOLM SKOVE, APPARAO RAO, Clemson University — We have studied the nonlinear dynamics of micro- and nano-cantilevers under varying ambient conditions using the Harmonic Detection of Resonance technique (HDR)1. In our studies, a cantilever is either microstructure shaped like a diving board, or a cantilevered MWNT. In this work, we report the dependence of the amplitude and Q of a silicon microcantilever (300 \(\mu\)m long, 35 \(\mu\)m wide, 2 \(\mu\)m thick) on ambient pressure. An environment of air at a pressure of \(10^{-3}\) Torr gives a high quality factor of \(\sim7000\). The response of higher harmonics of the ac voltage that drives the cantilever is also observed with varying chamber pressure. An investigation of the influence of ac and dc voltages on sensitivity shows very good agreement with a model calculation. The shift in the resonant frequency of cantilevers under different environments such as helium, air and argon at different pressures will be discussed. References: 1. J. Gaillard, M. J. Skove, R. Ciocan, and A. M. Rao, Rev. Sci. Instrum. 77, 073907 (2006). Contact Info: aaro@clemson.edu

11:27AM Y27.00002 Chemical and bio- sensor chips based on nanowires and carbon nanotube, CHONGWU ZHOU, FUMIAKI ISHIKAWA, USC — Significant effort has been devoted to the study of sensors using one-dimensional structured nanomaterials. Integration with other functionalities or combinatorial use of such sensors is a promising direction with which highly sophisticated functionalities can be realized. In this talk, we will present the use of the integrated/combined nano-chemical/bio sensors for more sensitive, precise, and selective sensing. We integrated micromachined heater into the chemical sensor based on In2O3 nanowire (NW), and the sensing experiments at the elevated temperatures demonstrated the detection of ethanol, which is undetectable at room temperature. Furthermore, combinational use of NW and carbon nanotube (CNT) chemical sensors combined with the micromachined heater were demonstrated toward the construction of electronic nose system. In addition, manufacturable multiplexed biosensor chips based on In2O3 NW, CNT, and aligned CNT were successfully fabricated with a highly generic strategy that can be extended to other one-dimensional materials. These sensors can be used as the platform for multiplexed sensing combined with selective functionalization.

11:39AM Y27.00003 Detection of adsorbed monolayers on suspended singlewalled carbon nanotubes, ZENGHUI WANG, JIANG WEI, WEI CHEN, ANDREW JONES, OSCAR VILCHES, DAVID COBDEN, University of Washington — Adsorbates on a suspended single-walled carbon nanotube at a coverage of one monolayer or less offer the opportunity to study the various phases and phase transitions of a system where the dimensionality is below two. This is because such a monolayer resembles a well studied 2D monolayer on planar graphite, but with a tight cylindrical boundary condition imposed. The adsorbed density for any gas can be measured by using the nanotube itself as a vibrating microbalance, whose frequency varies with the adsorbed density and whose amplitude is detected by the way it modulates the conductance. We are focusing on two systems both thoroughly studied before on 2D graphite: the noble gases Xe and Kr; and oxygen. The noble gases are attractive for their simplicity, and because in 2D they exhibit discontinuous phase transitions, which are not allowed in 3D according to an argument of Landau. They thus allow the possibility to confirm and explore this basic prediction of statistical mechanics for the first time. The magnetic and steric properties of phases of oxygen on 2D graphite, together with the question of its apparently unexplained large doping effect on nanotubes, make it particularly interesting and important. We have made suitable nanotube devices and will report on our progress in detecting monolayers on them.
11:51AM Y27.00004 Modeling of the Nonlinear Response of a Microcantilever: Understanding Higher Order Harmonics and Resonances. J.D. TAYLOR, JAY GALLIARD, MALCOLM SKOVE, APPARAO RAO, Clemson University. The most promising and readily scalable detection scheme for micro and nanocantilevers is electrostatic excitation and capacitive detection. This method has proven difficult to implement because of a large parasitic capacitance which masks the dynamic signal from the cantilever. Fortunately, the cantilever response exhibits several higher order harmonics and resonant peaks that can be exploited to avoid the parasitic capacitance and dramatically improve the signal to noise ratio. In this report a theoretical model of the cantilever response is presented that explains these higher order harmonics and resonances by considering nonlinear effects. Also, an experiment is presented in which the response of a microcantilever is measured simultaneously using laser reflectometry and capacitive techniques in order to separate the effects of current modulation and mechanical motion.

12:03PM Y27.00005 Sequence Dependent Single Stranded DNA-Single Walled Carbon Nanotube Interactions and Their Applications in Detection of Gaseous Analytes. SAMUEL KHAMIS, MICHELLE CHEN, ROBERT JOHNSON, A.T. CHARLIE JOHNSON, University of Pennsylvania. Recently there has been great interest in sensing strategies based on the use of non-covalent means to tune the chemical affinity of single walled carbon nanotube field effect transistors (SWNT FET’s). The combination of single-stranded DNA (ssDNA) and SWNT FET’s is particularly intriguing because of their chemical compatibility and diverse chemical recognition properties. We have demonstrated the utility of such devices for vapor sensing, and report here on results involving more than a dozen different ssDNA sequences. ssDNA/SWNT based sensors are sensitive to ppm’s of said gases, with response and recovery times on the scale of seconds. In tests involving a gas panel that includes explosives, neuro-toxins, and disease defining compounds, sensor response is specific to particular sequences of ssDNA. Given the extremely large number of different ssDNA sequences available, this observation opens up possibility of creating a large number of sensors with widely varying response characteristics, as required for an “electronic nose” system for the detection and classification of vapor mixtures. C. Staii, M. Chen, A. Gelperin, and A.T. Johnson, Nano Lett. 2005, 5, 1774-1778 This work supported by the JSTO DTRA and the Army Research Office Grant # W911NF-06-1-0462

12:15PM Y27.00006 Fabrication and characterization of individual nanotube based nanoelectrodes for chemical and biological sensing. KYUNG-SUK YUM, HANNA CHO, JIE HU, MIN-FENG YU, University of Illinois at Urbana-Champaign. We present the fabrication and characterization of individual nanotube based high aspect ratio nanoelectrodes for chemical and biological sensing. The nanoelectrodes are fabricated by coating nanotubes with metal and, subsequently, with insulating layers, and cutting the end of the nanotubes. This process yields ring-shaped nanoelectrodes with total structural diameter of ~100 nm, including insulating layers, and length up to ~30 μm. The nanoelectrodes are characterized by cyclic voltammetry (CV) and the structure of the nanoelectrodes is examined in transmission electron microscopy (TEM). The nanoelectrodes show steady-state voltammetric current responses and good insulation of the side wall of nanoelectrodes. These high aspect ratio nanoelectrodes will open up a new opportunity for electrochemical sensing in microscale environments, e.g. probing local intracellular environments without damaging cells, with high temporal and spatial resolution.

12:27PM Y27.00007 Electrical Detection of Protein Binding Using Carbon Nanotubes. M. CHEN, S.M. KHAMIS, S. DATTA, J.E. FISCHER, A.T. JOHNSON, U. of Pennsylvania, Y.-B ZHANG, M. KANUNGO, A.J. HO, P. FREIMUTH, D. VAN DER LELIE, B. PANESSA-WARREN, J.A. MISIEWICH, S.S. WONG, Brookhaven National Lab. For bio-molecular sensors, the swCN-FETs exhibit distinct electrical responses for specific and non-specific binding of molecules on the nanotube surface. Human receptor molecules are covalently functionalized onto the nanotube surface, while the electronic integrity of the nanotube is preserved. Then the adenosine, which binds specifically to the human receptor, is introduced to the swCN-FET functionalized with human receptor. The covalent binding between the adenosine and human receptor is detected through a significant decrease in the device current. Other molecules that do not bind specifically to the human receptor are also investigated as controls, and no current change is observed. Our findings have potential for sensitive detection and further understanding of virus infections in humans. Fundings: JSTO DTRA and the Army Research Office Grant # W911NF-06-1-0462, Laboratory for Research on the Structure of Matter (NSF DMR00-79909), and US Department of Energy, grant No. DE-FG02-98ER45701.

12:39PM Y27.00008 Transmission line impedance of carbon nanotube thin films for chemical sensing applications. G. ESEN, M. S. FUHRER, Department of Physics and Center for Superconductivity Research, University of Maryland, College Park, Maryland 20742, J. H. CHEN, M. ISHIGAMI, E. D. WILLIAMS, Laboratory for Physical Sciences and Department of Physics, University of Maryland, College Park, Maryland 20742. We measure the resistance and frequency-dependent (50 Hz - 20 KHz) gate capacitance of carbon nanotube (CNT) thin films as a function of DC gate bias under ambient conditions, in ultra-high vacuum, and under low-pressure (∼10⁻⁶ Torr) of analytes. This research was supported by the Laboratory for Physical Sciences and the U.S. Army Research Laboratory MICRA Program. MI received support from the Director of Central Intelligence Postdoctoral Fellowship program.

12:51PM Y27.00009 Harmonic Detection of ω₀/n Superharmonics in Microcantilevers via Electrostatic Actuation/ Detection. J. GAUILLARD, J. TAYLOR, G. KESKAR, M. SKOVE, A. RAO, Clemson University. In nonlinear dynamics, mechanical motion can be made up of a complicated mixture of vibrations. In resonating structures, nonlinearities are ubiquitous and more often than not are undesirable. On the other hand, nonlinear dynamics and chaos in electrostatic microelectro-mechanical systems (MEMS) has been shown to be useful for various applications, including secure communications, MEMS filters, and scanning force microscopy. Exploiting these dynamics opens the door for nanoelectromechanical systems (NEMS) by providing signals with higher quality factors and better signal-to-background ratios. In cantilever-based MEMS, the nonlinear dynamics usually stems from harmonically forced excitation in which only the second superharmonic has been theorized or detected. Here we measure the nonlinear effects. Also, an experiment is presented in which the response of a microcantilever is measured simultaneously using laser reflectometry and capacitive techniques in order to separate the effects of current modulation and mechanical motion.

1:03PM Y27.00010 Electromechanical Response of Single-wall Carbon Nanotubes to Torsional Strain in a Self-Contained Device. A. R. HALL, M. R. FALVO, R. SUPERFINE, S. WASHBURN, University of North Carolina at Chapel Hill. The response of single-wall carbon nanotube transport properties to applied shear strain has been measured. The strain is applied in a self-contained nanoelectromechanical device. We find that the measured resistance of an individual nanotube can increase or decrease depending on initial band structure, and that this change is approximately proportional to the applied strain.
1:15PM Y27.00011 Kinetics of Desorption of Oxygen, SHARVIL DESAI, University of Louisville, GAMINI SUMANASEKERA, Dept. of Physics, University of Louisville, CHAMINDA JAYASINGHE, University of Cincinnati, DAVID MAST, Dept. of Physics, University of Cincinnati — The kinetics of desorption of oxygen was studied by measuring in-situ thermopower of the Single Walled Carbon Nanotube samples subjected to (a) post synthesis acid treatment by refluxing (b) high temperature annealing at 10⁻⁷ Torr (c) plasma (Ar, O₂, H₂) treatment using an inductively coupled plasma reactor. Raman Spectroscopy and X-Ray Photoluminescence Spectroscopy were used to identify wall defects and other defects created due to each treatment on the nanotubes. Also we have estimated binding energy of oxygen with the carbon in all cases.

3 Corresponding Author

1:27PM Y27.00012 High-Performance ZnO Nanowire FETs, PAI-CHUN CHANG, ZHIYONG FAN, CHUNG-JEN CHIEN, JIA GRACE LU, University of Southern California — Zinc oxide (ZnO) nanowires have attracted tremendous interest due to their remarkable physical properties and versatile applications in electronic devices, such as logic circuit, UV emitter and photodetector, as well as chemical sensor. In the previous research report, ZnO nanowire configured as field effect transistor (FET) shows an electron mobility ranging from 3 to 80 cm²/V·s without surface treatments. In order to optimize the performance of devices, it is crucial to improve the carrier transconductance and mobility in the nanochannel. In our work, single-crystalline ZnO nanowires were synthesized via a catalyst-assisted chemical vapor deposition method. Temperature dependent photoluminescence measurements demonstrate the evolution of peak intensities resulted from different radiative mechanisms. The sharp peak with its full-width half maximum of 3.6meV at 12 K and the absence of other bound-exciton lines indicate that the as-grown nanowires are of high crystal and optical qualities. Following CMOS compatible procedures to passivate surface defect states and also to reduce chemisorption processes, the as-grown FETs exhibit orders of magnitude improvement in the on/off ratio, sub-threshold swing and field effect mobility. Remarkable mobility exceeding 4000 cm²/V·s was estimated.

1:39PM Y27.00013 N-doped carbon nanotubes and their behavior as ammonia sensors, ANTONIO J.R. DA SILVA, MARIANA ROSSI, FREDERICO D. NOVAES, A. FAZZIO, Instituto de Física - Universidade de São Paulo — CNx nanotubes can display a measurable variation in resistance upon exposure to ammonia. We present a microscopic model for the origin of these variations. We studied, using Total Energy DFT calculations, a (5,5) CNT containing pyridine-like N atoms replacing C atoms, and how the NH₃ molecule binds to these sites. We also investigate how these defects affect the transport charge properties using a Non-Equilibrium Greens Function formalism. We initially studied a defect composed by a vacancy surrounded by 3 pyridine-like rings. The most stable adsorption configuration for the ammonia molecule adsorbed close to this defect is dissociative, with an amino group (NH₂) fragment bound to one of the nitrogens and a H atom bound to another. This configuration leads to an increase in the conductance and cannot, therefore, explain the increase of resistance that has been experimentally observed. We then investigate a variety of other configurations in order to propose possible causes for the resistance increase. We find that a divacancy surrounded by 4 pyridine-like defects is the most stable N-defect, instead of the previously proposed one. The ammonia also dissociates into NH₂ and H. Moreover, the calculated change in conductance after the NH₂ dissociation has the correct trend when compared to the experimental results. We acknowledge FAPESP, CNPq and CENAPAD-SP.

2:03PM Y27.00015 Hydrogen Physisorption Properties of Single-Walled Carbon Nanotubes Studied by Soft-X-Ray Spectroscopy, J. ZHONG, LBNL and BSRF, Beijing, S. BARCELO, LBNL, J.-W. CHIOU, Tamkang Univ., C. L. DONG, Ins. of Phys., Taipei, C. L. CHANG, W.-F. PONG, Tamkang Univ., Y. Y. CHEN, Ins. of Phys., Taipei, S. MAO, LBNL, Z. Y. WU, BSRF, Beijing, J.-H. GUO, LBNL — Single-walled carbon nanotubes (SWNT) for nano gas sensors becomes a subject of active research. Different mechanisms for interaction of gas and SWNTs were reported. The electrical resistance was reported to change in a semiconductor SWNT when exposed to gases. The mechanism was interpreted to be collisions between gas molecules and tube wall. The major experimental effect is transport response to inert gases. It is said that deformation from collisions can change the electronic properties of SWNTs. So far there is few study to verify the mechanism and thus further investigation is needed. We have performed soft-x-ray absorption experiment to show the in-situ interaction between SWNTs and gas molecules under ambient temperature and pressure. The gas adsorption changes in electronic structure of SWNTs can be recovered by evacuation of gas. The collision of gas molecules to SWNTs can be responsible to the pressure-dependent spectral change. The raising gas pressure up to 10 torr induces deformation of SWNTs thus decreases the conductance, and further increase of pressure will recover the deformation due to inner tube collisions.


11:15AM Y31.00001 Magnetic Resonance Studies of Crystalline Ge₅Sb₂Te₃ and Sb₂Te₃₁, DAVID BOBELA, University of Utah, P. CRAIG TAYLOR, Colorado School of Mines — Recent technological applications of some chalcogenide materials, which are materials containing a group VI atom, have prompted studies of the local atomic structure of the amorphous phase. In particular, Ge₂Sb₂Te₅ has been employed as the prototypical phase-change memory material, since its structure can be rapidly switched from the crystalline phase to the amorphous phase with high fidelity. The metastability in the local bonding structure that produces this phase-change phenomenon is not yet understood. Magnetic resonance methods can be used to study local order as a function of the stoichiometry and phase of the material. As a starting point in understanding the magnetic resonance data for amorphous Ge₅Sb₂Te₃, we have used nuclear magnetic resonance and nuclear quadrupole resonance techniques to study crystalline Ge₅Sb₂Te₃ and Sb₂Te₃. We present estimates of the quadrupole coupling constants, and the asymmetry parameters of the electric field gradient for the ¹²¹Sb nuclei. The relationship between these parameters and the local atomic structure of crystalline Ge₅Sb₂Te₃ will be discussed. In particular, the Sb sites appear to depart from axial symmetry, a conclusion that is difficult to obtain from standard scattering experiments.

¹ AFOSR grant F29601-03-01-0229.
11:27AM Y31.00002 Terahertz Transmission Through Quasiperiodic Arrays of Subwavelength Apertures

TATSUNOSUKE MATSUI, Physics Dept., University of Utah, AMIT AGRAWAL, AJAY NAHATA, ECE Dept., University of Utah, Z. VALY VARDENY, Physics Dept., University of Utah — The extraordinary light transmission (EOT) through optically thick metallic films perforated with two-dimensional (2D) subwavelength hole array was originally explained in terms of resonant coupling to surface plasmon polaritons (SPPs) modes via grating coupling; and thus numerous EOT studies have been done on periodic hole arrays. Here we demonstrate terahertz EOT through 2D quasicrystalline array of subwavelength apertures that are not Bravais lattices, but, nevertheless of which structure factor shows discrete Fourier transform components. We found that such patterns also exhibit strong EOT bands indicating that SPP interaction also occur in quasiperiodic structures. This approach dramatically expands potential design parameters for aperture arrays and opens up exciting new avenues for optoelectronic devices, especially in the THz spectral range.

1This work was supported in part by a grant from the SYNERGY program at the University of Utah.

11:39AM Y31.00003 Terahertz Transmission Through Aperiodic Arrays of Subwavelength Apertures

AMIT AGRAWAL, ECE Dept., University of Utah, TATSUNOSUKE MATSUI, VALY VARDENY, Physics Dept., University of Utah, AJAY NAHATA, ECE Dept., University of Utah, ECE DEPT., UNIVERSITY OF UTAH TEAM, PHYSICS DEPT., UNIVERSITY OF UTAH TEAM — The recent surge of interest in the field of surface plasmon polaritons (SPPs) resulted in part following the initial demonstration of extraordinary optical transmission (EOT) through periodic arrays of subwavelength apertures. Ensuing experimental and theoretical studies on these and associated structures were focused primarily on periodic structures. In this submission, we demonstrate that aperture periodicity is not crucial for obtaining strong EOT resonances. We demonstrate this phenomenon by measuring the EOT of an aperiodic array of subwavelength apertures fabricated on free standing metal films in the terahertz spectral range. We observed sharp resonances in the transmission spectra at frequencies matching the aperture array ‘structure factor’. The aperiodic structures were designed using a general numerical approach for patterns in which no associated geometrical tiling rules exist.

1This work was supported in part by a grant from the SYNERGY program at the University of Utah.

11:51AM Y31.00004 Micro-Raman and FTIR Studies of Synthetic and Natural Apatites

A. ANTONAKOS, E. LIAROKAPIS, National Technical University of Athens, Greece, TH. LEVENTOURI, Florida Atlantic University, Boca Raton, FL, USA — B-type synthetic carbonate hydroxyapatite (CHAp), natural carbonate fluorapatite (CFAp) and silicon-substituted hydroxyapatite (SiHAp), have been studied by using micro-Raman and infrared (IR) spectroscopy. It was found that while B-type carbonate substitution predominates in carbonate apatites (CAPs), A-type is also detected in all types of apatites. B-type carbonate substitution causes a broadening of the $v_1$ P-O stretching mode that is associated with the atomic disorder within the phosphate tetrahedron. An $\sim 15$ cm$^{-1}$ shift of the $v_{33}$ P-O antisymmetric IR mode was observed upon heat-treatment of the CFAp to drive the carbonate off. This shift indicates that the P-O bond lengths on the mirror plane increase when carbonate leaves the apatite structure suggesting that carbonate substitutes on the mirror plane of the phosphate tetrahedra. The present results support the substitution mechanism proposed on the basis of neutron powder diffraction studies of the same samples. The intensity ratios of the $v_2$ IR CO$_3$ and $v_1$ PO$_4$ bands in samples with various carbonate contents provide a calibration curve for estimating the degree of carbonization of CAPs.

12:03PM Y31.00005 Propagation of Electromagnetic Waves in a One Dimensional Photonic Crystal with DPS/DNG Layers

JOSEPH SHAHBAZIAN, ARAM KARAKASHIAN, UML — Although materials having positive permittivity and permeability (DPS) are well known, recently electromagnetic materials with negative permittivity and permeability (DNG) have been given much attention. Wave propagation in a double negative medium and also photonic crystals has been studied analytically and experimentally. The material parameters are complex and frequency dependent to account for both dispersion and absorption. The real part of the corresponding index of refraction can be negative only in narrow frequency bands. Here we have studied theoretically the propagation of electromagnetic waves in a one dimensional photonic crystal composed of alternating layers of DNG and DPS layers. We find that this type of photonic crystal in the visible wave range exhibits negative refraction in a wider frequency range.

12:15PM Y31.00006 NMR Studies of Ba$8$Al$_x$Ge$_{46-x}$ and Ba$8$Ga$x$Ge$_{46-x}$ Clathrates

GOU WEIPING, YANG LI, JI CHI, V. GORUGANTI, K. D. D. RATHNAYAKA, JOSEPH H. ROSS, JR., Department of Physics, Texas A&M University — We have prepared a series of clathrates of the general form, $\text{Ba}_8\text{Al}_{x}\text{Ge}_{46-x}$. X-ray measurements indicate that Al occupies predominantly the 24$k$ site, similar to previous observations for the Ga analogs. $^{13}$N MR measurements using wide-line and MAS spectrometers indicate two different local Al sites, one with a relatively small quadrupole splitting, attributed to the 24$g$ site, and one with a larger quadrupole splitting attributed to Al adjacent to a vacancy. We also discuss the results of $\textit{ab-initio}$ calculations supporting these conclusions. $T$-dependent NMR relaxation results show roughly Korringa-type behavior for both series of compounds for $x < 16$, characteristic of heavily-doped semiconducting materials. The lowest-carrier density Ga$_{16}$ sample shows changes in $T_1$ and Knight shift characteristic of incipient localization at low temperatures, however analysis indicates that the carriers remain in the regular band rather than forming an impurity band. For Ga$_{x}$ clathrates synthesized from excess Ga, the NMR $T_1$ changes abruptly, indicative of a change in band-edge symmetry for $p$-type material. This work was supported by the Robert A. Welch Foundation (grant A-1526) and the National Science Foundation (DMR-0103455).

12:27PM Y31.00007 Thermodynamics of type-I and type-II Si clathrates: a computer simulation study

CAETANO MIRANDA, MIT, ALEX ANTONELLI, Universidade Estadual de Campinas — Few years ago a guest free type-II clathrate of silicon was obtained. This new form of elemental silicon is remarkably stable up to high temperatures. It is now clear that in order to devise new synthesis routes for these materials a better understanding of their thermodynamic properties is highly desirable. In this work, we present a computational study, employing the isobaric Monte Carlo method, of the thermodynamic properties at zero pressure of different phases of silicon, namely, both clathrate forms, $\text{Si}_{16a}$ (type-I) and $\text{Si}_{34b}$ (type-II), diamond crystalline silicon, liquid silicon, and amorphous silicon ($\alpha$-Si). The Gibbs free energies, calculated by the reversible scaling method, allow us to determine the stable and metastable relations between these various phases. We have found the melting point of $\text{Si}_{16a}$ and $\text{Si}_{34b}$ clathrate structures to be at $1892 \pm 25$ K and $1522 \pm 25$ K, respectively. Our result for the melting point of $\text{Si}_{34b}$ is in good agreement with the experimental value of 1473 K. The results also indicate that both clathrate forms are more stable than $\alpha$-Si for any temperature up to their melting point. Based on our findings we discuss the feasibility of routes for the growth of these materials, such as solid-phase epitaxy and liquid-phase epitaxy.

1Financial support from FAPESP, CNPq, and FAEP-UNICAMP
Spire Corporation, Bedford, MA 01730 showed no wear, to potentially extend lifetimes by orders of magnitude in industrial or biomedical applications.

1:39PM Y31.00008 Dielectric spectroscopy of pulsed laser deposited type Pb(Zr,Ti)O$_3$ (PZT)/CoFe$_2$O$_4$ (CFO) and CFO/ PZT multilayers thin films. NORA ORTEGA, University of Puerto Rico, I. TAKEUCHI, University of Maryland — Multiferroics are a novel class of next generation multifunctional materials. Intensive research is being pursued towards the development of materials with high magneto-electric (ME) coupling. In case of composite thin films, ferromagnetic (FM) columns epitaxially grown in ferroelectric (FE) matrix, exhibit large ME coefficient compared to multilayers structures. From the studies it appears that the distribution of FM phase in FE matrix plays an important role to obtain high ME effect. In the present work we fabricated composite thin films of FE Pb(Zr,Ti)O$_3$ (PZT) and FM CoFe$_2$O$_4$ (CFO) multilayers with 3, 5 and 9 layers PZT/CFO (PC) and CFO/PZT (CP) by pulsed laser deposition. We have investigated the effect of reversing the order of FE and FM layers in the multilayer configuration on the properties. The TEM and XPS depth profile of the films, showed that the layer structure was not maintained. The dielectric constant of PC and CP multilayers showed strong frequency dispersion. Reversing the multilayers configuration from CP to PC resulted in increasing the remanent polarization. The observed dielectric relaxation has been explained by Maxwell-wagner type contributions. The ME effect of multilayer films will be discussed.

12:39PM Y31.00009 Measurement of the DC resistance of thin film semiconductor-gas systems: comparison to the effective medium approximation$^1$. J. GARNER, B. CARRICO, J. SAREDY, J. TRACY, N. PATEL, University of North Florida — DC resistance measurements have been made of a thin film semiconductor (indium tin oxide) that has been exposed to various gases (acetylene, methane, and sulfur dioxide). Our motivation is to use the time-dependent resistance as a means of identifying unknown gases. Three transport models were used to compare to the measurements: a simple resistor network model, a dynamic Maxwell-Garnett theory (DMGT), and a dynamic effective medium approximation (DEMA). The latter two theories are dynamic because the volume fractions of the constituents of the thin film-gas composite vary with time during the gas adsorption process. The resistor network model gives the general trend of the data. This novel application of the DMGT and DEMA yield results that are nearly identical to each other and that are in good agreement with our measurements.

1:03PM Y31.00010 Functionally graded, nanocrystalline, multiphase, B- and C-based superhard coatings. CHARLES BLATCHLEY, Pittsburgh State University, KS 66762, FEREYDOON NAMAVAR, University of Nebraska Medical Center, Omaha, NE 68198, ERIC TOBIN$^1$, JOHN ADAMS, Spire Corporation, Bedford, MA 01730, MICHAEL GRAHAM, Northwestern University, Evanston, IL 60208 — Candidate ceramic coatings for bearing applications must meet several criteria, such as hardness, to limit abrasive damage. Adhesion is essential to prevent destructive three-body wear. Toughness helps avoid brittle fracture and coating failure. Finally, temperatures during deposition must not damage the substrate. We report fabrication and testing of functionally-graded, nanocrystalline, multiphase Ti/BN coatings by ion beam assisted deposition (IBAD), with these properties. Hardness was measured >42 GPa. Structural grading transitions from metallic to covalent bonding through the film, controlling constituents (TiN, TiB$_2$, B$_4$C, BN) to optimize adhesion, internal stress, hardness, and wear resistance. Pin-on-disk wear testing for 5 million cycles at 1 GPa contact stress, showed no wear, to potentially extend lifetimes by orders of magnitude in industrial or biomedical applications.

1:15PM Y31.00011 Photoemission Studies on Bulk Amorphous Steels. MICHAEL BUETTNER, University of Virginia, Materials Science & Engineering, B. SIMON MUN, Advanced Light Source, Lawrence Berkeley National Laboratory, PETER OELHAFEN, University of Basel, Institute of Physics, PETRA REINKE, University of Virginia, Materials Science & Engineering — The recent availability of bulk amorphous metals (BMGs) promises interesting new applications for the near future based on the superior structural, physical, and chemical properties of such materials compared to conventional steels. In order to shed light on local atomic and electronic structure photoemission studies have been performed on BMGs containing Fe, Cr, Mo, C, B, and Er. Progressing from ternary to penternary alloys we studied changes in the local electronic environment in a systematic manner by means of core-level and valence band spectroscopy. Step-by-step ion irradiation revealed differences in surface and bulk elemental composition and bonding. In particular the bonding state of B changes from oxide (surface) to boride (bulk). Iron exhibits the most prominent spectral changes of all the metal constituents, showing significantly higher core-level binding energies in penternary alloys than in ternary and quaternary compounds. Investigations of the Fe 3s multiplet splitting indicates a dependence of the splitting energy on the abundance of erbium in the alloy. Future experiments will focus on bulk material properties by preparing alloy surfaces in vacuum and addressing the constituents’ chemical environment in more detail.

1:27PM Y31.00012 Nanoscale Order in Marginal and Bulk Amorphous Metal Alloys$^1$. PAUL VOYLES, WILLIAM STRATTON, JINWOO HWANG, JOSEPH HAMANN, HONGBO CAO, JOHN PEREPNZKO, Y. AUSTIN CHANG, Materials Science and Engineering, University of Wisconsin, Madison — Using fluctuation electron microscopy (FEM), we have shown that both an Al-based marginal amorphous Al alloy, Al$_8$Y$_2$Fe$_5$, and a Zr-based bulk amorphous alloy, Zr$_{54}$Cu$_{18}$Al$_{28}$, have significant nanoscale structural order at a length scale of ~1.5 nm. In both cases, that order can be reduced by annealing below $T_g$. In the Al alloy, this order is associated with proto-crystalline clusters formed in the liquid or during the rapid quench. The size and/or density of these clusters can also be modified by small additions of Cu and Ti. The nature of the structure in the Zr alloy has not been determined, but our results show that statistical relaxation on aging, which in bulk metallic glasses is commonly understood in terms of redistribution of free volume in the form of atom-size voids, involves rearrangements of groups of ~10-100 atoms.

1:39PM Y31.00013 Strain localization in disordered materials and implications for constitutive laws for sliding interfaces. MARY LISA MANNING, JAMES S. LANGER, JEAN M. CARLSON, University of California Santa Barbara — We investigate localization in a model for disordered materials such as granular particles or plastically deforming asperities that are sheared between sliding interfaces. We model the dynamics of configurations of particles that are more susceptible to deformation under shear stress using Shear Transformation Zone (STZ) theory. STZ theory has recently been modified to include effective disorder temperature dynamics, which provides a mechanism for strain softening and shear localization because as the material is strained it becomes more disordered and a more disordered material is more susceptible to deformation. The STZ effective temperature model is investigated in a simple shear geometry by numerically integrating the equations of motion and analyzing their generalized stability. We find that a material with a spatially homogeneous initial effective temperature distribution (corresponding to a slowly quenched sample) supports homogeneous flow, but one with a finite spatial perturbation in the disorder (corresponding to a rapidly quenched sample) develops a shear band, which leads to a dramatic reduction in the yield stress and a modified constitutive law for the interface.

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$^2$This work is supported by Office of Naval Research, US DOD #N000140610133.

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A comparison between defects created by light soaking and tritium decay in amorphous silicon, TONG JU, University of Utah, STEFAN ZUKOTYNSKI, NAZIR KHERANI, University of Toronto, P. CRAIG TAYLOR, Colorado School of Mines, PAUL STRADINS, National Renewable Energy Laboratory, UNIVERSITY OF TORONTO COLLABORATION — We compare two ways to create defects in a-Si:H, namely decay of bonded tritium and irradiation with visible light. Tritium decays to He\(^3\), emitting a beta particle and an antineutrino. In tritium doped a-Si:H samples each beta decay of tritium bonded to silicon will create a defect by converting a bonded tritium to an interstitial helium, leaving behind a silicon dangling bond. We track these defects using electron spin resonance (ESR). We have kept the sample in liquid nitrogen for two years. After two years the defect density increases without saturation to a value of \(7 \times 10^{19} \text{cm}^{-3}\). In the second experiment, we have kept the sample in liquid nitrogen irradiated with white light of intensity about 100mW/cm\(^2\). After about 6 months, the spin density increased to about \(9 \times 10^{17}\text{cm}^{-3}\) with no evidence of saturation. In the tritiated sample the increase in the defect density is proportional to the time, \(t\), while in the light-soaked sample the increase is approximately proportional to \(t^{1/3}\). This difference in behavior will be discussed.

Effective Mass Density of Fluid-Solid Composites, JUN MEI, Department of Physics, Hong Kong University of Science and Technology, Hong Kong, China, ZHENGYOU LIU, Department of Physics, Wuhan University, Wuhan, China, WEIJIA WEN, PING SHENG, Department of Physics, Hong Kong University of Science and Technology, Hong Kong, China — We show through rigorous derivation and experimental support that the dynamic effective mass density of an inhomogeneous mixture, used in the prediction of wave velocities in the long wavelength limit, can differ from the static version—the volume average of the component mass densities. The physical reason for this difference is explained. The dynamic mass density expression, first derived by Berryman more than two decades ago, is shown to give a closer correspondence between the acoustic and electromagnetic metamaterials by allowing for negative mass densities at frequencies around resonances.