Electronic Materials and Processing
Room: Dona Ana - Session EM+MI-MoA

Semiconducting and Highly Correlated Oxides

Moderator: L.J. Brillson, The Ohio State University

2:00pm **EM+MI-MoA1 Oxide Superconducting Semiconductors**, ***H.Y. Hwang***, University of Tokyo, Japan **INVITED**

$SrTiO_3$ is the lowest density known bulk superconductor [1]. In addition, it is a dielectric material which is well-known for its very large low-temperature dielectric constant, arising due to the proximity of a ferroelectric instability [2]. With recent advances in complex oxide heteroepitaxy, these physical properties provide a unique opportunity to apply concepts of band structure engineering to this superconducting semiconductor.

At the conducting $LaAlO_3/SrTiO_3$ interface, the superconducting state can be back-gate modulated to induce a 2D superconductor-insulator transition [3]. Using magnetotransport studies in the normal state, we find that the mobility variation is five times as large as the change in sheet carrier density [4]. These results indicate that the relative disorder strength increases across the superconductor-insulator transition, which can be understood to be driven by localization as in previous examples of ultra-thin quenched amorphous superconductors such as Bi [5].

Using heterostructures of $Nb:SrTiO_3$ embedded in undoped $SrTiO_3$, we have studied the crossover from 3D to 2D superconductivity as the thickness of the doped layer is decreased. A notable feature is that the mobility increases in the 2D limit to over 6 times the highest bulk value at comparable doping, in analogy to delta-doping in semiconductors. This aspect suggests that a new regime of 2D superconducting phase transitions can be accessed approaching the clean limit, in contrast to the dirty limit seen at the back-gated $LaAlO_3/SrTiO_3$ interface [6].

This work was done in collaboration with Y. Kozuka, C. Bell, M. Kim, S. Harashima, Y. Hikita, and B. G. Kim.

[1] J. F. Schooley *et al.*, Phys. Rev. Lett. **12** (1964) 474.

[2] K. A. Mueller and H. Burkard, Phys. Rev. B **19** (1979) 3593.

[3] A. D. Caviglia *et al.*, Nature **456** (2008) 624.

[4] C. Bell *et al.*, Phys. Rev. Lett. **103** (2009) 226802.

[5] A. M. Goldman and N. Markovic, Physics Today **226** (1998) 39.

[6] Y. Kozuka *et al.*, Nature **462** (2009) 487.

3:00pm **EM+MI-MoA4 X-ray Photoemission Spectroscopy of Sr_2FeMoO_6 Film Stoichiometry and Valence State**, ***M.M. Rutkowski***, *A.J. Hauser, F.Y. Yang, R. Ricciardo, T. Meyer, P.M. Woodward, A. Holcombe, P.A. Morris, L.J. Brillson*, The Ohio State University

4:00pm **EM+MI-MoA7 Electronic Structure of Ferrimagnetic $Co_{1-x}Fe_{2+x}O_4$ Determined by Soft X-ray and Ultraviolet Spectroscopies**, ***J.A. Moyer***, *C.A.F. Vaz,* Yale University, *D.A. Arena,* Brookhaven National Laboratory, *V.E. Henrich*, Yale University

Developing new materials with large spin polarizations, high Curie temperatures and resistivities similar to those of semiconductors would greatly benefit the field of spintronics. Cobalt ferrite ($CoFe_2O_4$), like its parent compound magnetite (Fe_3O_4), is a promising material for spintronic applications due to its high Curie temperature (T_c=793 K) and large predicted spin polarization; however, $CoFe_2O_4$ is an insulator. Cobalt ferrite becomes an *n*-type conductor when doped with excess iron – $Co_{1-x}Fe_{2+x}O_4$; the origin of the conduction is electron hopping between Fe^{2+} cations in octahedral sites. The strong localization of electrons on the Fe^{2+} cations in this highly correlated oxide keeps the conductivity in the semiconducting range. In this work, heteroepitaxial $Co_{1-x}Fe_{2+x}O_4$ thin films have been grown on MgO (100) and $MgAl_2O_4$ (100) and (110) with *x* ranging from 0 to 0.5. The electronic band structure near the Fermi energy is measured with ultraviolet photoelectron spectroscopy (UPS), and the results are correlated with resistivities determined from transport measurements. This range of doping allows for the resistivity to be tailored over two orders of magnitude. The cation valence states and occupation sites are determined with x-ray photoelectron spectroscopy (XPS) and x-ray absorption spectroscopy (XAS). Bulk magnetic moments are obtained with SQUID magnetometry, while bulk and site specific orbital and spin magnetic moments are obtained using x-ray magnetic circular dichroism (XMCD). The XMCD measurements provide a view of the spin polarization of the Fe^{2+} octahedral cations responsible for conduction. The wide variety of measurements enables us to determine the electronic structure of $Co_{1-x}Fe_{2+x}O_4$, an important development for the goal of determining the viability of $Co_{1-x}Fe_{2+x}O_4$ as a spin-polarized source or detector in spintronic devices.

This research is primarily supported by NSF Grant MRSEC DMR-0520495.

4:20pm **EM+MI-MoA8 Effects on the Electronic Band Structure of EuO Films upon Gd Doping**, ***J.A. Colón***, *J. An, K.D. Belashchenko,* University of Nebraska - Lincoln, *Y.B. Losovyj,* Louisiana State University, *P. Liu, X.J. Wang, J. Tang,* University of Wyoming, *P.A. Dowben*, University of Nebraska - Lincoln

High quality films of EuO and Gd doped EuO were successfully grown on Si (100) via pulse laser deposition (PLD). The addition of 4% Gd introduces considerable affects the texture growth direction, although the crystal structure remains intact. This Gd doping also have a strong influence in the electronic structure of these films, in particular the apparent band offsets, making the material appear considerably more n-type in combined photoemission and inverse photoemission studies. There are also concomitant changes to the conductivity properties. To further elucidate the influence of Gd doping on the electronic band structure of the EuO films, heterojunction devices were constructed resulting in diodes with very distinct properties a negative differential current that depends on magnetic field.

4:40pm **EM+MI-MoA9 Catalytic Performance for Soot Combustion of Lanthanum-Based Cobalt-Iron Perovskite Materials**, ***L.M. Petkovic***, *S.N. Rashkeev,* Idaho National Laboratory, *V. Utgikar*, University of Idaho

Perovskite-type oxide materials with a general formula La0.8A0.2Fe(1-y)Co(y)O(3-delta), where A is Sr or Ba and y=0.4 or 0.5, were prepared and tested in the combustion of carbon black, which can be regarded as a conservative soot model. Maximum combustion rates under temperature programmed combustion conditions were found at temperatures about 150°C lower than blank combustion experiments. A combination of density-functional-theory (DFT) calculations and characterization analyses such as surface area, infrared spectroscopy, X-ray diffraction, and temperature programmed oxidation and reduction were applied to elucidate the main processes that contribute to the activity of these catalysts for soot combustion. The results suggest the importance of the kinetics of oxygen adsorption and reaction at the surface and oxygen migration in the bulk.

Actinides and Rare Earths Topical Conference
Room: Isleta - Session AC+MI-TuM

Actinide and Rare Earth Magnetic Interfaces & Nanostructures

Moderator: T. Durakiewicz, Los Alamos National Laboratory

8:20am **AC+MI-TuM2 An Alternative Model for Electron Correlation in Pu**, *S.W. Yu, J.G. Tobin,* ***P. Soderlind***, Lawrence Livermore National Laboratory

Using a density functional theory based approach that treats the 5f electrons relativistically, a Pu electronic structure with zero net magnetic moment is obtained, where the 5f orbital and 5f spin moments cancel each other. By combining the spin and orbital specific densities of states with state, spin and polarization specific transition moments, it is possible to reconstruct the experimentally observed photoemission spectra from Pu. Extrapolating to a spin-resolving Fano configuration, it is shown how this would resolve the extant controversy over Pu electronic structure. See J. Phys.: Condens. Matter 20 (2008) 422202 for more detail. Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344. This work was

supported by the DOE Office of Science, Office of Basic Energy Science, Division of Materials Science and Engineering.

8:40am **AC+MI-TuM3 Correlation Effects in Gadolinium Compounds: Comparison of Theory and Experiment**, ***P.A. Dowben***, University of Nebraska - Lincoln **INVITED**

The apparent Gd 4f binding energy in photoemission spectroscopy is strongly affected by both correlation energy contributions, and final state effects in photoemission. The latter are clearly strongly influenced by metallicity and screening [1]. To understand these various contributions to the observed electronic structure of gadolinium compounds, we compare a series of studies on gadolinium compounds and clusters with pure and alloyed gadolinium films [2]. These materials range from the metallofullerenes, in which a metal atom or cluster is encapsulated inside a fullerene, such as in the "buckyball" C60, to more conventional rare earth compounds like GdN, Gd2O3, Gd doped HfO2 and Gd-Ni alloys. The Gd3+ ion exhibits bonding and hybridization that is quite different for these various compounds. While the total spin multiplicity of Gd is maximum because of its half-filled 4f state, and the atomic orbitals are strongly hybridized with the C60 molecules in the example of Gd@C60 [3] or oxygen in the case of Gd doped HfO2 [4], while the highest possible symmetry site for gadolinium is generally not favored. These results are to some extent a confirmation of theoretical expectations but there are complications. There is experimental evidence for intra-atomic hybridization with both the unoccupied and occupied Gd 4f states, as well as band dispersion even for the occupied Gd 4f states in some systems [2] and spin dependent screening [5].

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[2] T. Komesu, H. K. Jeong, David Wooten, Ya. B. Losovyj, J. N. Crain, M. Bissen, F. J. Himpsel, J. Petrosky, Jinke Tang, Wendong Wang, I.N. Yakovkin, and P. A. Dowben, *Physica Status Solidi* B **246** (2009) 975-980

[3] R. F. Sabirianov, W. N. Mei, Jing Lu, Y. Gao, X. C. Zeng, R.D. Bolskar, P. Jeppson, Ning Wu, A.N. Caruso, and P. A. Dowben, J. Phys. Cond. Matter 19 (2007) 082201

[4] Ya. B. Losovyj, I. Ketsman, A. Sokolov, K. D. Belashchenko, P.A. Dowben, J. Tang, Z. Wang, *Appl. Phys. Lett.* **91** (2007) 132908

[5] Hae-Kyung Jeong, R. Skomski, D. Wisbey, P.A. Dowben, *Physics Letters* A **341** (2005) 508-515

This work has been undertaken with Y. Losovyj, T. Komesu, Hae-Kyung Jenong, I. Ketsman, N. Wu, A. Sokolov, J. Colon Santana, W. Choe, K. D. Belashchenko, R. F. Sabirianov, W. N. Mei, Jinke Tang, A.N. Caruso, D. Wooten, R. Skomski, F. Himpsel, E. Vescovo

9:20am **AC+MI-TuM5 Electronic Phase Diagram of Rare Earth Mono-Pnictides and Mono-Chalcogenides**, ***L. Petit***, *R. Tyer,* Daresbury Laboratory, UK, *A. Svane,* Aarhus University, Denmark, *Z. Szotek, W.M. Temmerman*, Daresbury Laboratory, UK **INVITED**

The self-interaction corrected local spin density (SIC-LSD) approximation is used to predict the ground state valency configuration of the manifold of rare earth mono-pnictides and mono-chalcogenides. This is a first-principles methodology that adequately describes the dual character of f-electrons, itinerant vs. localized, and the goal is to combine it with high throughput computing, in order to achieve predictive capability in the search for and design of new materials with specific physical properties. For the rare earth mono-pnictides and mono-chalcogenides we predict an electronic phase diagram composed of metallic, semi-conducting and heavy fermion like regions, and exhibiting valency transitions brought about by a complex interplay between ligand chemistry and lanthanide contraction. Our findings, including the ground state lattice parameters, and the "intermediate valent" character of compounds such as SmO and TmSe, are in excellent agreement with the available experimental data.

10:40am **AC+MI-TuM9 Nanotechnology in the Actinides: Uranium Thin Films and Multilayers**, ***R.S. Springell***, University College London, UK **INVITED**

From the modern scientific landscape of nanotechnology research, the manipulation of elements and compounds on a near-atomic scale has contributed to innovations, some of which affect our everyday life. The growth of thin films and multilayers has allowed systematic studies of reduced dimensionality and the electronic interplay between dissimilar materials. Important applications have emerged, notably the GMR effect1. However, such studies of systems containing actinide elements are, to our knowledge, absent, but offer exciting possibilities because of potential hybridization involving the 5*f* electronic states.

The samples are prepared by a dedicated sputtering facility at Oxford University, UK2.

Our investigation into uranium multilayers, which involves both bulk as well as element specific techniques, compares the structural properties2 and electronic interactions3,4,5 of uranium interleaved with layers of ferromagnetic Fe, Co, Ni, and Gd. Only in the case of U/Fe is a large magnetic moment induced on the U atoms, close to the interface5.

The study of epitaxial uranium films is initially concerned with the nature of the structural constraints incurred by the substrate and buffer6 and the potential for stabilizing structures otherwise absent in the bulk. a–U (which is the normal ambient orthorhombic phase) grows well on a Nb buffer on sapphire. In the bulk it exhibits a charge-density wave (CDW) at 43 K, so in epitaxial films an interesting question is the minimum thickness for the CDW to appear; we have already observed the CDW down to 10 nm. Using epitaxial *hcp*–Gd as a buffer, we have produced *hcp*–U for the first time7. The observed $c/a = 1.90$ is larger than for any other hexagonal element. We report also our first efforts to prepare epitaxial UO2 films.

11:20am **AC+MI-TuM11 Growth and Characterization of Dy/Y Superlattices**, *J. Yu, H. Sato, P.R. LeClair,* ***G.J. Mankey***, University of Alabama, *J.L. Robertson, R.S. Fishman*, Oak Ridge National Laboratory

Inelastic neutron scattering is the world's most powerful tool to study the magnetic excitations of solids. We aim to study spin wave dispersion relations in multilayer structures and how they are affected by the indirect RKKY exchange interaction through nonmagnetic spacers. Dy was chosen as the magnetic film since it has a huge magnetic moment of 10.2 Bohr magnetons and the neutron scattering cross section is directly proportional to the atomic moment. For elastic scattering, a film with thickness of order 100 nm is sufficient, but inelastic neutron scattering has a considerably lower cross-section requiring much more material for measurement. To enable such a study, many samples with tightly-controlled thickness and crystallinity must be fabricated. The neutron experiments can then be performed by stacking 8-10 samples, each with 50-100 superlattice repeats. The number of repeats for each sample is limited by the accumulation of defect structures over the growth front. Using a home-built sputtering system, we have achieved the ability to make suitable samples. The system has computer-controlled magnetron sputtering guns and a sample tranfer system which enables continuous sample rotation of a 2" diameter wafer at 900ºC during sputtering in an ultra-pure environment. Maintaining a good vacuum is essential since both Y and Dy are highly reactive and form stable

oxides with only a minute amount of oxygen in the sputtering environment. In addition, the dispersion relations of the spin wave modes are highly sensitive to thickness variations, so it is essential to create samples with uniform and repeatable layer thicknesses. We report the growth and characterization of epitaxial Dy/Y multilayer samples and our optimization of the growth temperature to produce samples with well-defined superlattice Bragg peaks in high-angle x-ray diffraction.

Funded by US-DOE through DE-FG02-08ER46499 and research at Oak Ridge National Laboratory's High Flux Isotope Reactor was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

11:40am **AC+MI-TuM12 Study of f Electron Correlations in Uranium- and Cerium-Oxides by BIS and XES**, ***S.W. Yu***, *B.W. Chung,* Lawrence Livermore National Lab, *D.G. Waddill,* Missouri University of Science and Technology, *J.G. Tobin*, Lawrence Livermore National Lab

When a high energy electron beam impinges on a material, some electrons of the incident electron beam are decelerated into the unoccupied states of the material with a spontaneous emission of electromagnetic radiation (bremsstrahlung). This bremsstrahlung process can be considered as the inverse of the photoemission process if the initial and final states are exchanged and the occupied state is replaced by the unoccupied one. BIS (Bremsstrahlung Isochromat Spectroscopy) is a very powerful tool to study the bulk unoccupied electronic structures of materials, minimizing the impact of surface effects.

Recently, we have developed a BIS capability, using an XES-350 system from VG SCIENTA, at the Lawrence Livermore National Laboratory, to investigate the electronic structure of actinides, in which 5f electrons play important roles to determine their physical and chemical properties. Similar to the resonant photoemission, the measured BIS signal can be resonantly enhanced when the electron energy reaches the threshold of the binding energy of a core electron, as a result of the interference between the BIS signal and the x-ray emission signal emitted by a radiative decay of the core hole. In case of cerium-oxide, the BIS signal is enhanced significantly at the 3d→ 4f resonance. However, in the case of uranium-oxide, the BIS signal is enhanced only slightly at the 4d → 5f resonance.

The x-ray emission can be described as a spontaneous emission of photons in a transition that are allowed by the dipole selection rules between two electronic states. The implication of the dipole selection rules is that, for example, in the case of K-emission, where 1s holes are created, only states with p-character are allowed to decay and the partial p-type density of state is measured in a x-ray emission spectrum. Therefore, the x-ray emission spectra from a variety of core levels allow us to study the symmetries of the occupied electronic states.

We will present the resonant BIS spectra and x-ray emission spectra (U 4f, 4d, O1s, Ce 3d) of the uranium- and cerium-oxides. Based on these data, we will discuss the detailed electronic structures of f electrons in uranium- and cerium-oxides.

Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under contract DE-AC52-07NA27344. This work was supported by the DOE Office of Science, Office of Basic Energy Science, Division of Materials Science and Engineering.

Magnetic Interfaces and Nanostructures
Room: Zuni - Session MI+EM-TuA

Spintronics
Moderator: S.-W. Hla, Ohio University

2:00pm **MI+EM-TuA1 All-Electric Spintronics with Quantum Point Contacts: From Spin Physics to Spin Electronics**, ***P. Debray***, University of Cincinnati **INVITED**

The controlled creation, manipulation, and detection of spin-polarized currents by purely electrical means remains a central challenge and objective of spintronics. One approach to meet this challenge has been to rely on coupling of the electron orbital motion to its spin. Attempts have been made to use the Rashba spin-orbit coupling as a tool to achieve this objective. Despite intense effort there has so far been no report of any success. In this talk, I will present experimental evidence that a quantum point contact made from a semiconductor with intrinsic spin-orbit coupling can generate completely spin-polarized current when its lateral confinement is made highly asymmetric by tuning the bias voltages of the side gates that create it. Such quantum point contacts can be used as all-electric spin polarizer or detector. I will discuss how they can replace the ferromagnetic electrodes of conventional spin valves to yield all-electric spin valves with very high On/Off values. By avoiding the use of ferromagnetic contacts or external magnetic fields, the use of such quantum point contacts will make feasible the development of a variety of semiconductor spintronic devices.

2:40pm **MI+EM-TuA3 Incorporation of Mn Atoms into N-polar Wurtzite GaN(000-1) Surface Studied using Scanning Tunneling Microscopy**, ***A.V. Chinchore***, *K. Wang, M. Shih, A.R. Smith*, Ohio University Nanoscale and Quantum Phenomena Institute

There has been much interest in dilute magnetic semiconductors. Mn-doped gallium nitride was proposed as a possible dilute magnetic semiconductor with Curie temperature above room temperature [1]. Consequently, many studies have been carried out to investigate the growth and properties of Mn-doped GaN. Despite much work however, not much is known about the location of Mn atoms in the GaN surface. We present in this new study evidence for the precise position of Mn atoms in the nitrogen polar wurtzite GaN (000-1) surface.

The N-polar GaN (000-1) surface is prepared by molecular beam epitaxy using a Ga effusion cell and a rf N-plasma source on sapphire substrates. The growth is monitored in-situ using reflection high energy electron diffraction. The as-grown GaN surface shows a smooth 3×3 reconstruction. The sample is transferred in-situ to the analysis chamber where it is imaged using room-temperature scanning tunneling microscopy (STM). The as-grown sample surface shows large terraces of 3×3 reconstruction. Transferring the sample back to the growth chamber, Mn is then deposited onto the 3×3 surface at a rate of about 0.01 monolayers (ML's) per second for a total of about 0.3 ML, at a sample temperature of 250 ˚C. After this, the surface remains in a 3×3 structure.

STM images of the surface after Mn deposition show a modified 3×3 reconstruction including almost uni-axial trench-like structures over large areas which are not seen on the clean GaN surface. The closely-spaced trenches run along [11-20], and they are separated by an even number of gallium adlayer rows. The position of these features also coincides precisely with Ga adlayer row positions. A model for this structure involving Mn atoms within the GaN(000-1) adlayer has been developed. Additional work exploring the coverage dependence of this structure is also underway. This work has been supported by DOE (Grant No.DE-FG02-06ER46317) and NSF (Grant No.0304314). Equipment support from ONR is also acknowledged.

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3:00pm **MI+EM-TuA4 Formation of Ferromagnetic MnGa Monolayers on GaN(0001) Studied by STM**, ***K. Wang***, *A.V. Chinchore, M. Shi, A.R. Smith*, Ohio University Nanoscale and Quantum Phenomena Institute

Ferromagnetic (FM) metal/semiconductor bilayers are of great interest due to their importance in novel spintronics applications, such as spin injection and spin light-emitting diodes[1]. It has been shown[2] that δ-MnGa, a FM alloy with T_C higher than room temperature (RT), can be grown epitaxial on top of w-GaN(0001) with sharp interface and controllable magnetism. Here we report detailed studies on the formation of the first few MnGa monolayers formed by depositing up to 3 monolayers (ML's) of Mn onto w-GaN(0001) "1x1" surface at elevated substrate temperature. Mn-induced surface reconstructions and formation of smooth Mn_xGa_{1-x} crystalline monolayer films are observed by reflection high-energy electron diffraction (RHEED), Auger electron spectroscopy as well as in-situ RT-scanning tunneling microscopy (RT-STM). RHEED data showed well-ordered surface reconstructions exhibiting mainly 1/3rd and 2/3rd order streaks along [1-100] directions at lower than around 0.5 ML of Mn coverage, while two different sets of reconstruction streaks could be identified depending upon the Mn coverage. Two different types of atomic row-like features both running along close-packing direction of GaN, but having different row-row spacings, are observed with STM at room temperature. The unit-cells derived are consistent with RHEED observation. At higher than around 0.5 ML, atomically smooth MnGa layers start to cover up the surface as shown by both RHEED and STM; the epitaxial relationship is derived as d-MnGa[011]//GaN[0001] and d-MnGa[001]//GaN[11-20]. Structural and electronic properties at representative stages will be presented, as well as possible magnetic properties of MnGa ML's. This work has been supported by DOE (Grant No.DE-FG02-06ER46317) and NSF (Grant No. 0730257). Equipment support from ONR is also acknowledged.

[1] S.A. Wolf *et al*, Science **294**, 1488 (2001).

[2] E. Lu *et al*, Phys. Rev. Lett. **97**, 146101 (2006); K.K. Wang *et al,* Mater. Res. Soc. Symp. Proc. 1118-K06-06 (2009).

4:40pm **MI+EM-TuA9 Chemical Switching of Coupled Molecular Spins: On and Off**, *C. Waeckerlin, D. Chylarecka, A. Kleibert, K. Mueller,* Paul Scherrer Institute, Switzerland, *C. Iacovita,* University of Basel, Switzerland, *F. Nolting, T.A. Jung,* ***N. Ballav***, Paul Scherrer Institute, Switzerland

Herein we present a unique approach to reversibly control between the *on* and *off* state of the spin of an organometallic molecule coupled to a ferromagnetic substrate by a chemical switch. Such an ultimate degree of control was achieved via modification of the coordination strength of the central metal ion of the organometallic molecule by an external ligand. Thus the regulation of oxygen affinity in hemoglobin by iron-porphyrin moiety as shown in nature has been used as a designed concept to perform the switching event of single molecular spin. Use of external stimuli to control single molecular spins at magnetic-interfaces is of potential interest for spintronics and quantum information.

5:00pm **MI+EM-TuA10 The Spin-Resolved Electronic Structure of the Strongly Correlated $M^{II}[TCNE]^{\bullet-}$ Magnets**, *S.J. Janjua,* University of Missouri-Kansas City, *K.I. Pokhodnya,* North Dakota State University, *J. Trunk,* Brookhaven National Laboratory, *C.S. Olson,* North Dakota State University, *J.C. Sutherland, E. Vescovo,* Brookhaven National Laboratory, ***A.N. Caruso***, University of Missouri-Kansas City

$M^{II}[TCNE]^{\bullet-}$ organic-based magnets are an important class of solids for both application and magnetic exchange and correlation study. The detailed spin polarized occupied electronic structure of $M^{II}[TCNE]^{\bullet-}$ magnets has eluded description from conventional ligand field theory, the results of elementally- or spin-sensitive photon and electron spectroscopies as well as spin resolved density functional calculations. This talk will present heuristic models for M=V, Fe and Ni in the context of the local physical structure and recent less conventional electronic structure studies (UV/Vis MCD), but with a new twist to the onsite and nearest neighbor Coulomb repulsion based correlation.

In Situ Microscopy and Spectroscopy Topical Conference
Room: Acoma - Session IS+AS+NS+MI-WeM

In Situ Microscopy/Spectroscopy – In Situ Nanoscale Processes
Moderator: A. Mkhoyan, University of Minnesota

8:00am **IS+AS+NS+MI-WeM1 Low-dimensional Superconductivity of Pb Nanostructures**, ***J. Kim***, *H. Nam, G.A. Fiete, C.K. Shih*, The University of Texas at Austin

The influence of low-dimensional geometries on superconductivity is an important issue to study because in low dimensions it is key to understanding coherence and robustness of the superconducting state in quantum-mechanically confined geometries. The lateral size dependence of superconductivity on 2 dimensional Pb islands is studied by using *in-situ* low temperature Scanning Tunneling Microscopy/Spectroscopy (STM/S). The superconducting transition temperature (T_c) of each island is obtained by fitting the STS data with a BCS-like density of states. It is found that superconductivity shows a clear dependence on the Pb island lateral size even when it is larger than the bulk coherence length (~80nm), and it is also found that T_c drops very quickly below a certain lateral size. In addition, an intriguing lateral proximity effect is observed at the interface of different local superconducting regions of Pb islands. Current imaging tunneling spectroscopy (CITS) is used to visualize this proximity effect in real space.

8:20am **IS+AS+NS+MI-WeM2 Enabling the Measurement of In-Situ, Site-Specific Mineral Transformation Rates in Supercritical CO_2 through Development of a High Pressure AFM**, ***S. Lea***, Pacific Northwest National Laboratory, *S.R. Higgins,* Wright State University, *K.G. Knauss,* Lawrence Berkeley National Laboratory, *K.M. Rosso*, Pacific Northwest National Laboratory

8:40am **IS+AS+NS+MI-WeM3 Au on VLS-grown Si Nanowires: Spreading of the Liquid Metal Seed**, *E. Dailey, P. Madras,* ***J. Drucker***, Arizona State University **INVITED**

In situ TEM shows that liquid AuSi spreads from the seed along the NW sidewalls to form a thin liquid sheath for some growth conditions. The thin liquid film phase separates to form small solid Au clusters when the NW is cooled below the solidus temperature. Quantitative composition maps show that the Au composition is highest near the NW tip. The thickness and length that the liquid film spreads from the seed is growth condition and NW diameter dependent and represents a steady state during growth. These observations can be related to the spreading thermodynamics of liquid droplets along cylinders. Growth conditions for which the liquid AuSi spreads from the seed stabilize 'vertical' growth along <111> by lowering the surface energy of the high-energy {112} bounding facets. In contrast, the NWs kink toward <112> when grown using conditions that favor growth with Au-free sidewalls since these NWs are bound by facets that are found on the Si equilibrium crystal shape.

9:20am **IS+AS+NS+MI-WeM5 Advanced Study of Nanoscale Mechanisms: Plans for In-Situ TEM Microreactor, Gas Cell, and Multi-Beam Irradiation Experiments**, ***B.G. Clark***, *K. Hattar,* Sandia National Laboratories, *D. Nackashi, J. Damiano, S. Mick,* Protochips, Inc., *B.L. Doyle*, Sandia National Laboratories

Over the years, in-situ TEM experiments have allowed for observation of material mechanisms at high resolution and in real time; a feat often not possible with any other experimental technique. With increasing demand for understanding nanoscale material mechanisms, both with growth in the applications of nanomaterials and in the development of predictive materials models based on experimental observation, the realm of in-situ TEM experiments has continued to expand. Highlighted in this presentation will be the development of three, exciting new capabilities for in-situ TEM experiments at Sandia National Labs.

The first part of the talk will focus on the development of two new in-situ TEM stages. Expanding on the success of static and single inlet-outlet liquid cells, we are designing a new in-situ TEM microreactor liquid cell with the capability to mix fluids in controlled temperature regimes, to view reactions as a function of time, and to capture and analyze reaction products. Research programs using this stage will pursue studies of self-assembly, directed assembly, and nanoparticle formation and growth. In addition, for observation of advanced degradation of materials in the presence of gases and/or vapor, a new in-situ TEM gas cell stage is being developed. This stage will have the capability to study a variety of gas-solid and vapor-solid interactions, such as corrosion, oxidation, and hydriding, with accurate control over temperature and pressure. Envisioned research will include understanding environmental degradation of materials during storage of spent nuclear fuels, an issue of critical importance for the future of nuclear energy.

The second part of the talk will highlight the development of a new, triple-ion-beam in-situ irradiation TEM. By combining expertise in in-situ TEM experiments with expertise in ion beam studies, planning is currently underway that would culminate in the construction of an instrument capable of studying the effects of bombardment by up to three ion beams simultaneously within the TEM. This unique, triple-ion-beam capability would enable advanced experiments such as real-time studies of neutron induced damage and transmutation in a fission/fusion reactor by combining Fe, He, and H ions.

*This work is supported by the Division of Materials Science and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:40am **IS+AS+NS+MI-WeM6 *In Situ* TEM Investigation into the Thermal Stability of Nanograined FCC Metals and Alloys**, ***K. Hattar***, *B.G. Clark,* Sandia National Laboratories, *J. Kacher,* University of Illinois at Urbana-Champaign, *J.A. Knapp, D.M. Follstaedt, L.N. Brewer,* Sandia National Laboratories, *I.M. Robertson*, University of Illinois at Urbana-Champaign

Nanostructured materials often display very unique properties related to their far-from-equilibrium nature. Due to these unique structures, many of these materials transform into other, more stable microstructures with minimal thermal excitation. This work will highlight examples of the unexpected routes taken during the microstructural evolution of pulsed-laser deposited (PLD) free-standing face-centered cubic (FCC) thin films as a function of deposition condition and annealing temperatures. A direct comparison between the grain growth dynamics observed during *in situ* TEM annealing experiments in PLD films of high-purity aluminum, copper, gold and nickel films, as well as aluminum-alumina alloys shows a multitude of kinetics. For high-purity systems film thickness, void density, grain size distribution, and deposition temperature were found to be the primary factors observed controlling the rate, extent, and nature of the grain growth. The growth dynamics ranged from nearly classical normal grain growth to abnormal grain growth resulting in a bimodal grain size distribution. The grain growth rate was found to be highly dependent on the materials system despite all of the films being nanograined FCC metals produced by similar PLD parameters. The investigation of the aluminum-alumina alloys produced under various compositions and deposition parameters suggests that particle pinning can be used to maintain nanostructured films, even after annealing treatments at high homologous temperatures.

In addition to investigating the grain growth dynamics and the resulting grain size distribution, the variety of internal microstructures formed from thermal annealing were evaluated. These structures ranged from intergranular voids to stacking-fault tetrahedra. An unexpected, metastable hexagonal-closed packed phase was indentified in the high-purity nickel films. These *in situ* TEM observations have provided key insight into the microstructural evolution of nanograined free-standing metal films and the defect structure present in the grains resulting from various growth dynamics, in addition to suggesting multiple methods to tailor the structure and the resulting properties of nanostructured free-standing films.

*This work is supported by the Division of Materials Science and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy both at Sandia and under grant DE-FG02-07ER46443. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

10:40am **IS+AS+NS+MI-WeM9 In Situ TEM Studies of Nanomagnetism and Thermal Transport**, ***J. Cumings***, University of Maryland **INVITED**

The transmission electron microscope is a powerful tool for many areas of nanoscience. The combination of high spatial resolution and high time resolution, giving video-rate imaging, makes it uniquely capable of many types of studies of phenomena in-situ during imaging. Here I will present two areas where we have made recent advances. In nanomagnetic

structures, it is possible to image in real-time the reversal process of coupled systems called artificial spin ice. These systems exhibit frustration, leaving disorder in their lowest energy magnetic configurations. I will present studies showing the magnetic reversal processes for these structures, revealing that microscopically correlated events lead to avalanche phenomena. A second topic that I will present is electron thermal microscopy of carbon nanotubes. Here, a new technique will be introduced that allows thermal imaging with nanoscale spatial resolution. This technique has been used to study the thermal transport through carbon nanotubes, and I will present results showing that thermal contact resistance can limit the thermal transport in nanotubes. I will show that this contact resistance can be tuned by two orders of magnitude by appropriately controlling the fabrication of the contacts. Together these results serve to demonstrate the capabilities of studies utilizing in-situ transmission electron microscopy.

11:20am **IS+AS+NS+MI-WeM11 In-situ Infrared Transmission Analysis of Atomic Layer Deposition Reactions on Polymer Films and Fibers**, ***G.N. Parsons***, *B. Gong, J.S. Jur, C. Oldham, K. Lee*, North Carolina State University

Many new product applications related to packaging, filtration, protection and others offer substantial opportunities and raise new demands for polymer/inorganic thin film integration and surface modification. In-situ transmission infrared spectroscopy can provide critical insight into reaction mechanisms that proceed during inorganic film deposition on organics. We are particularly interested in low-temperature atomic layer deposition (ALD) which ideally proceeds through a binary sequence of self-limiting surface reactions to form highly conformal and uniform films on high surface area structures. In-situ IR spectroscopy allows us to probe and identify specific polymer/precursor reaction mechanisms that occur during precursor and reactant exposure. Typical atomic layer deposition precursors and reactants include trimethylaluminum (TMA), diethyl zinc (DEZ) and water, and polymer materials studied to date include polypropylene, polyamide-6, polyesters (such as polybutylene terephthalate), cellulose, polyvinyl alcohol and others. We have investigated deposition reactions on planar polymer sheets as well as micro- and nano-scale polymer fibers.

In-situ IR transmission data demonstrates that typical non-reactive materials such as polypropylene will take up precursors with minimal precursor/polymer reaction, resulting in subsurface alumina nucleation. Polymers with more reactive backbone or side chain groups, such as cellulose, polyvinyl alcohol or polyamide-6 react readily with the precursor. For example, when polyamide-6 is exposed to TMA, N-H and C-O stretching modes decrease markedly, indicating that TMA attacks the electrophilic carbon atom in the carbonyl group leading to methyl insertion and formation of C-O-Al- and C-CH_3 bonds. Electron micrograph images of polyamide fibers after TMA exposure confirms significant extent of reaction. Deposition on cellulose cotton fibers, however, shows primarily surface adsorption, resulting in true ALD growth and highly conformal film coatings by TEM. We will show details of the in-situ transmission ALD reactor, and illustrate how the tool is especially amenable and adaptable to in-situ surface reaction analysis on polymer fiber networks.

Magnetic Interfaces and Nanostructures
Room: Zuni - Session MI-WeA

Spintronic Devices and Proximity Effects
Moderator: R.A. Lukaszew, College of William and Mary

2:00pm **MI-WeA1 A New Twist on Spin Devices**, ***S. Wolf***, University of Virginia **INVITED**

The use of a spin polarized current to rotate the magnetization direction of a ferromagnetic has a number of important implications for novel magnetic devices. Spin torque can switch the resistivity of a magnetic tunnel junction, create spin waves over a very wide range of frequencies, and move magnetic domain walls. I will describe some of the recent advances in Spin Torque Magnetic Random Access Memory (STT-RAM), spintronic nano-oscillators and flux shuttle memory. In addition I will describe a very novel logic array based on electrical control of magnetism called a Reconfigurable Array of magnetic Automata which uses the ferroelastic strain on a magnetic nanopillar to rotate the direction of magnetization. I will show how this can be used to perform logic at very low power approaching zeptojoules per switch..

2:40pm **MI-WeA3 Thermal Stability and Switching Distributions in Nanoscale Spin Torque Transfer Random Access Memory Devices**, ***S.E. Russek****, R. Heindl, W.H. Rippard, M.R. Pufall, T. Cecil*, NIST-Boulder

Thermal stability and switching distributions of MgO magnetic tunnel junction (MTJ) devices, that are being developed for spin-torque-transfer random access memory (STT-RAM), have been modeled using single domain simulations. The simulations incorporate realistic current-voltage characteristics, a field-like torque term and thermal heating. These elements are required to allow the single domain model to fit data from standard STT-RAM devices. Simulations were performed with a stochastic thermal field with 10,000 repetitions for each value of applied current and pulse duration. For a typical STT-RAM device with dimensions of 50 nm x 150 nm, at room temperature, with a 10 ns pulse width, the write error rate (WER = 1- switching probability) falls off at a rate of 40 mV/decade. To achieve a write error rate below 10-9, which is a typical value for current memory, the switching voltage must be 360 mV above the intrinsic switching voltage. The direction of the spin polarizer was systematically varied and it was found that switching probability decreases as the polarizer is moved off the device easy axis. The fall off in WER with pulse amplitude remained roughly constant.

The simulations are compared to data from devices consisting of a Co40Fe40B20 free layers, 1.1 nm MgO tunnel barrier, and a synthetic antiferromagnetic fixed layer. The average resistance area product (RA) and tunneling magnetoresistance (TMR) are RA=5 Ohm micrometer2 and TMR=150%, respectively. The devices were patterned using e-beam lithography and ion beam etching into ellipsoids of sizes ranging between 50 nm x 150 nm to 100 nm x 300 nm (all with aspect ratios 1:3). The devices were imbedded in a high frequency coplanar wave guide structure to allow high-speed switching and high-frequency thermal ferromagnetic resonance (FMR) measurements. The high speed switching measurements confirmed that simple thermally activated switching modelscannot accurately fit the measured data. The single domain simulations, with a field like torque term and thermal heating, can replicate several key features of the measured switching distribution. The thermal FMR data, however, often show a complex mode structure indicating that the real devices deviate considerably from simple single domain behavior.

These results indicate that slow fall off of the WER may be a key problem for STT-RAM technology. Within the single domain model, the slow fall off of the WER is intrinsic. To obtain a more rapid fall off in the WER, micromagnetic design concepts must be employ to prevent the device from accessing low torque configurations during the switching process.

3:00pm **MI-WeA4 Growth and Magnetism of Mn-nanostructures Embedded in a Group IV Semiconductor Matrix**, ***K.R. Simov***, University of Virginia*, C.A. Jenkins, M. Liberati,* Lawrence Berkeley National Laboratory*, P. Reinke*, University of Virginia

The magnetic doping of the group IV semiconductors Si and Ge with Mn is coveted as valuable component in novel spintronics devices. Their magnetic doping is hampered by the low solubility of Mn in both elements, and the formation of silicide and germanide phases which modify or suppress the magnetic response of the material. We therefore investigate Mn-nanostructures which are synthesized on the Si(100)(2x1) surface and then capped with a layer of Si or Ge to protect the integrity of the nanomaterial. The Mn-nanostructure is therefore embedded as a delta-doped layer within a group IV semiconductor matrix.

The first section of our presentation focuses on nanostructure synthesis, in particular the growth of monoatomic Mn-wires on the Si(100)(2x1) surface, where the dimer row structure guides the wire formation. A scanning tunneling microscopic (STM) study establishes the relation between the nanostructure type and the quality of the substrate, which is expressed in the concentration of defects prior to Mn deposition. An increasing defect concentration (1.0 % to 18.2%) leads to a suppression of wire formation and the growth of ultrasmall Mn-clusters is favored, which allows for an excellent control of nanostructure type. Surface structuring through the presence of dimer vacancy lines, or narrow terraces offer an additional route to control Mn-wire formation. A Monte-Carlo based model is introduced to describe the surface processes which lead to wire-formation.

The second section of our presentation assesses the stability of the nanostructures during the growth of the Si or Ge caps. The capping of nanostructures is indispensible for preservation of the nanostructures' unique capabilities in devices, and is critical for magnetic measurements such as VSM (vibrating sample magnetometry) and XMCD (X-ray magnetic circular dichroism, Advanced Light Source, Lawrence Berkeley National Laboratory). An STM observation of the growth process of the Si and Ge caps shows that the Mn-nanostructures are indeed preserved, and we are therefore able to assess the magnetic properties of Mn-wires and ultrasmall clusters.

The third section of our presentation is devoted to the discussion of the magnetic properties of the Mn-wire and Mn-cluster structures. The role of magnetic anisotropy, the ionic and metallic contributions from the Mn-nanostructure, and the nature of the magnetic coupling within the respective nanostructure, and with the cap-material will be discussed.

The support from NSF-Chemistry and DOE are gratefully acknowledged.

4:00pm **MI-WeA7 Exchange Bias Using Ideal Antiferromagnets**, ***D. Lederman***, West Virginia University **INVITED**

Exchange bias is the interaction at the interface between an antiferromagnetic material and a ferromagnetic thin film or nanoparticle which causes the center of the ferromagnetic hysteresis loop to shift away from zero field, effectively resulting in a unidirectional anisotropy. Despite the fact that this effect was discovered approximately fifty years ago, and that it is used in magnetic sensors found in hard drives, the fundamental mechanism responsible for this interaction was poorly understood until recently. Important advances using ideal antiferromagnets (antiferromagnets with well understood and relatively simple properties) have been made during the past few years to assess or validate theories that explain exchange bias. My group has used transition metal difluoride epitaxial thin films, such as $Fe_xZn_{1-x}F_2$ and $Fe_xNi_{1-x}F_2$, which allow us to vary the magnetic disorder and anisotropy of the antiferromagnet in a controlled manner. Traditional magnetometry techniques, as well as more sophisticated experiments sensitive to the depth profile of the magnetization, such as x-ray magnetic circular dichroism (XMCD) and polarized neutron reflectivity (PNR), have allowed us to understand the interface processes responsible for the effect. I will discuss the important results from these experiments, including 1) the effects of short range order at the surface of the antiferromagnet above its Néel temperature; 2) the observation of pinned and unpinned magnetic moments at the ferromagnet/antiferromagnet interface; and 3) the effects of the magnetic anisotropy of the antiferromagnet on the temperature dependence of the exchange bias and the possibility of reversing the effect at low temperatures.

This work was supported by the National Science Foundation.

4:40pm **MI-WeA9 Spintronic Effects in Molecular Materials: The Past, Present, and Future**, ***G.J. Szulczewski***, The University of Alabama **INVITED**

In this talk I will introduce the general concepts of spintronics and highlight some of the key experimental results that have catalyzed the emerging research area known as "organic spintronics". The confluence of spin-electronics, which combines transition metal ferromagnets and inorganic semiconductors, and molecular-electronics, which combines organic semiconductors and non-magnetic metals, has lead to the evolution of organic spintronics. Furthermore, the development of organic light emitting diodes and organic photovoltaic cells has proven that molecular thin films can reliably function as the active layer in commercial products. Consequently it often envisioned that spin dependent conduction in organic-based semiconductors, rather than traditional charge transport, can be

manipulated and detected to fabricate low-power, non-volatile, multifunctional devices because electron spin coupling to orbital angular momentum and nuclear spin is weak. Recent experimental evidence is beginning to demonstrate this view is too simplistic and hyperfine coupling is very important in the hopping transport mechanism characteristic of disordered organic semiconductors.

The focus of this talk will be on the phenomena of magnetoresistance; specifically in vertical device structures with conducting electrodes used to separate an organic semiconductor layer(s). In many laboratories around the world such devices are observed to change resistance when placed in an external magnetic field. If both electrodes are magnetic and the change in the resistance corresponds to the coercive fields of the electrodes, then the magnetoresistance can be interpreted as spin-polarized injection, transport, and ejection of carriers from one ferromagnetic layer, through the non-magnetic spacer layer, and into the second ferromagnetic layer, respectively. However, when neither of the electrodes is magnetic the magnetoresistance must arise some other phenomena and there are several competing theories to describe the effects. The bulk of this talk will be devoted to reviewing case studies from the former class of devices, since there are well-accepted criteria to support the interpretation of device magnetoresistance when using magnetic electrodes. In addition I will cite examples where the interfaces of the devices have been examined by surface sensitive spectroscopy/microscopy techniques and correlated to device performance. Finally I will conclude by recommending some new experiments that could reveal more knowledge of the fundamental spintronics effects in molecular materials and suggest some possible applications.

5:20pm **MI-WeA11 Probing Induced Magnetism in Vanadium Nano-islands on Cr by Spin-polarized STM**, ***C. Clavero***, College of William & Mary, *M. Bode,* Argonne National Laboratory, *G. Bihlmayer, S. Blügel,* Institut für Festkörperforschung, Germany, *R.A. Lukaszew*, College of William & Mary

The growth mode and magnetism at V(001)/Cr(001) interfaces are still controversial and in recent years have attracted considerable theoretical and experimental interest since they strongly affect the properties of multilayered structures prepared with these materials. Both V and Cr are *bcc* 3*d* transition metals with approximately half-band filling. Cr exhibits antiferromagnetism along the <001> direction which converts the (001) surfaces to ferromagnetic (001) planes that couple antiferromagnetically from layer to layer. Interestingly, it has been theoretically predicted that a single V layer on Cr couples antiferromagnetically to Cr with an induced V moment of 2.1 μ_B/atom, but drastically reducing the Cr magnetic moment[1]. Previous reports using Mössbauer spectroscopy[2] applied to Cr/V multilayers have given direct experimental evidence for a reduction of the Cr magnetic moment near the interface region. In addition, recent neutron scattering experiments have shown that proximity effects in Cr/V multilayers lead to the appearance of a 50 Å magnetically dead Cr layer near the interfaces[3].

Despite the interest in V/Cr(001) interfaces, possible magnetic polarization of V by proximity to the antiferromagnetic Cr(001) substrate has not been yet fully investigated. We report on our spin-polarized scanning tunneling microscopy (SP-STM) studies on subatomic layer coverings of V on Cr(001) substrates and experimentally demonstrate antiferromagnetic coupling between V islands and the Cr(001) underlying surface. V was evaporated on Cr(001) substrates under ultra-high vacuum conditions (base pressure in the low 10-11 mbar) and at 250 ºC, temperature reported as optimum to achieve high quality multilayers with abrupt interfaces2. V coverages ranging from 0.1 to 1.5 atomic layers (AL) where explored. Antiparallel coupling between the V islands and the Cr(001) substrate is found, with the magnetic contrast disappearing when the V islands start to coalesce for increasing coverages starting at 0.9 AL. In addition, using Scanning Tunneling Spectroscopy and density functional theory calculations, it was found that during the early stages of growth the islands exhibit radial symmetry in their chemical composition, with Cr-rich composition in the center and V-rich regions at the rims. Interestingly, for higher coverages such islands coalesce evidencing an island assisted interface alloying mechanism.

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Magnetic Interfaces and Nanostructures
Room: Zuni - Session MI+TF-ThM

Magnetic Nanostructures, Thin Films and Heterostructures
Moderator: C. Clavero, College of William & Mary

8:00am **MI+TF-ThM1 AC Susceptibility of Ni Bars with Magnetic Single Domain**, *X.G. Zhang, I.I. Kravchenko, S.T. Retterer, J.F. Wendelken,* ***Z. Gai***, Oak Ridge National Laboratory

For thin films, the generalized Curie-Weiss law extends the power law scaling well above Tc by replacing the linear reduced temperature t_L by a nonlinear reduced temperature t_{NL}=1-Tc/T. The film thickness d and temperature T are usually not independent variables in the scaling. Using the nonlinear reduced temperature, the power law scaling was shown to be accurate over the entire paramagnetic regime [1-3]. However, at low temperature, thermally activated domain wall motion is expected to contribute significantly to the temperature dependence of magnetic properties, therefore the scaling law is generally believed not to extend far below Tc. Such belief was contradicted by a very recent experiment [4] that showed a surprising power law scaling for the in-plane susceptibility of sputtered Ni films deposited on silicon for the entire temperature range between zero and Tc. In addition, thickness and temperature dependence are completely decoupled. This scaling result implies that even in the ferromagnetic regime, there is no domain wall motion contribution to the low field susceptibility [4]. To clarify the role of domain wall motion, arrays of single domain Ni microstructures are studied experimentally and theoretically. We will show the results of the AC susceptibility measurements of Ni microstructures with magnetic single domain, in which the contributions of domain wall motion and spin fluctuation to the susceptibility are separated.

This research at Oak Ridge National Laboratory's Center for Nanophase Materials Sciences was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

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8:20am **MI+TF-ThM2 Deuterium Absorption in Co/Pd Multilayers**, ***K. Munbodh***, *F.A. Perez, D. Lederman,* West Virginia University, *M. Zhernenkov, M. Fitzsimmons*, Los Alamos National Laboratory

The absorbed concentration of deuterium was calculated in Co/Pd multilayers at standard temperature and pressure using in-situ neutron reflectometry. The out-of-plane film expansion and deuterium concentration-depth profiles were determined from the fitting of the neutron reflectivity data. The measurements demonstrated that deuterium is absorbed in all the Pd layers. However, the concentration of the hydrogen varies with Pd layer thickness. Polarized neutron reflectometry with applied field of 6.5 kOe in the plane of the sample was performed and the detailed magnetic depth profile was established. These results showed an overall increase in magnetization upon deuterium absorption.

8:40am **MI+TF-ThM3 Correlated Structural and Magnetic Studies of Capping and Seed Layer Dependent Epitaxial FePd Thin Films**, ***L. Wang***, *J.R. Skuza,* College of William & Mary, *T. Mewes,* University of Alabama, *C. Clavero, R.A. Lukaszew*, College of William & Mary

FePd binary alloys can form a chemically ordered phase ($L1_0$) that exhibits interesting properties such as high perpendicular magnetic anisotropy (PMA). This property has drawn great attention for many technological applications such as ultrahigh density magnetic recording media and spin transfer torque random access memory (STT-RAM). We investigate the influence of different capping layers (Au, Pd and V and compare with an insulating capping layer such as MgO) on the magnetic properties, particularly the magnetic anisotropy and damping, of highly anisotropic $L1_0$ FePd films which were grown onto MgO (001) substrates using magnetron sputtering in an ultra-high vacuum deposition system. We use x-ray diffraction techniques to study the chemical ordering of the films, and vibrating sample magnetometry (VSM), magnetic force microscopy (MFM) and ferromagnetic resonance (FMR) to investigate the magnetic properties. Our aim is to investigate and tailor the structural and magnetic properties of highly ordered FePd thin films with strong PMA via adequate choice of capping and seed layer materials.

We thank W. Chen and S. A. Wolf for their collaboration. Funding for this project was obtained from NSF grants DMR 0804243 and DMR 0605661 and a Cottrell Scholar Award from the Research Corporation.

9:00am **MI+TF-ThM4 Microstructural, Magnetic Anisotropy, and Magnetic Domain Structure Correlations in $L1_0$ Ordered Thin Films**, ***J.R. Skuza***, *L. Wang,* College of William & Mary, *W. Chen, J. Lu,* University of Virginia, *T. Mewes,* University of Alabama, *C. Clavero, R.A. Lukaszew*, College of William & Mary

Understanding microstructural, magnetic anisotropy, and magnetic domain structure correlations in materials with strong perpendicular magnetic anisotropy (PMA) is of fundamental interest and it is also important in many technological applications such as next generation magneto-recording, magneto-optical, and patterned media. The $L1_0$ ordered phase of some binary alloys (FePt, FePd, MnAl, etc.) has strong PMA due to chemical ordering that can be controlled with adequate thin film deposition parameters and/or subsequent thermal annealing treatments. A detailed structural (XRD and AFM) and magnetic (MFM, SQUID, and FMR) study on two of these $L1_0$ ordered alloys will be presented. Epitaxial FePd thin films with various capping layers were grown by dc magnetron sputter deposition onto MgO(001) substrates. A quantitative analysis and correlation of the strong PMA to magnetic domain structure in these FePd films was accomplished with good agreement using an analytical energy model [1]. MnAl thin films were grown by reactive biased target ion beam deposition onto MgO(001) substrates. Effects of the growth conditions and subsequent thermal annealing treatments on the microstructure and magnetic properties will be discussed.

This work was supported by the Virginia Space Grant Consortium, National Science Foundation (DMR Grants #0355171, #0605661, and #0804243), the American Chemical Society (PRF Grant #41319-AC), and the Research Corporation Cottrell Scholar Award. K. Yang, B. Wincheski, and S. A. Wolf are acknowledged for their collaboration.

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9:20am **MI+TF-ThM5 Correlating Microstructure with Magnetic Properties Variation in Patterned Magnetic Nanostructures with Transmission Electron Microscopy**, ***J.W. Lau***, National Institute of Standards and Technology **INVITED**

Patterned magnetic nanostructures are keystone components in technologies such as hard drive media, sensors, and the magnetoresistive device variants (read-head, random access memory, logic). During manufacturing, different processes produce defects that are the source of variations in magnetic properties in magnetic nanostructures. One example is the Co/Pd nanodot array, interesting for its potential in realizing the bit-patterned media data storage platform. We showed that grains of a particular orientation formed during the film deposition can act as trigger sites for magnetization reversal. Therefore, the ease of switching a particular nanodot among millions of nominally identical nanodots depends on the random presence of trigger grains within it. When considered as an ensemble, the nanodot array will exhibit a switching field distribution; this is the superposition of the individual switching fields unique to each nanodot. In general, switching field distribution and other magnetic property variations in patterned magnetic nanostructures can present major problems for devices development where uniform magnetic performances are required.

The fact that magnetic phenomena in patterned magnetic nanostructures, whether it be magnetization reversal or magnetoresistance, are always observed as distributions means that it is import to identify the root causes to these distributions. An essential aspect to furthering the progress in developing magnetic nanostructure devices is therefore, to correlate nanostructure, defects and interfaces, and chemical composition to magnetic behaviors on the nanoscale. To this end, one of our main focuses is in developing ways to measure variations in magnetic properties using transmission electron microscopy (TEM). TEM is one of the few tools that can provide structural, chemical and magnetic information all at the same time.

In this presentation, I will highlight specific examples of measurements developed for patterned magnetic nanostructures using a TEM. The first example is the microstructure correlation to the switching field distribution in Co/Pd nanodots, described earlier. The second example is a set of *in situ* tunneling measurements where we succeeded in measuring unique energy barrier height and tunneling magnetoresistance (TMR) on fully functional nano-magnetic tunnel junctions (MTJ) built as a TEM sample. Finally, I

will show how single nanostructure magnetometry can be achieved within a TEM.

10:40am **MI+TF-ThM9 Partial Perpendicular Anisotropy of CoFeB with Vanadium Capping**, ***A. Natarajarathinam***, *Z.R. Tadisina, S. Gupta*, University of Alabama

Magnetic tunnel junctions with vanadium-based capping layers on top of the CoFeB free layer have been studied. The interest in the effect of capping on the free layer originated from reports[(1)] that cap layers influence the crystallization of the CoFeB free layer through diffusion of the B into the cap, as well as induce a partial perpendicular magnetic anisotropy (PPMA or PPA) in the free layer[(2,3)]. Different cap layers differently accelerate the diffusion of the B from the free layer. In this study, we have sputter-deposited V/Ru and V/Ta capping layers on CoFeB and subsequently characterized these films by magnetometry and ferromagnetic resonance (FMR). We have found that V/Ru and V/Ta capping of CoFeB induces partial perpendicular anisotropy (PPA) in CoFeB, as well as reduces the Gilbert damping parameter, confirming results reported by other researchers[(4)]. The origin of this PPA is believed to be caused by the interface anisotropy between the free layer and the capping layer. The effect of post-deposition annealing, CoFeB thickness, and doping of CoFeB with vanadium on the anisotropy and damping of these V/Ru and V/Ta capped samples has been studied for the free layers. Doping CoFeB with vanadium greatly reduces the $4\pi M_s$ and $4\pi M_{eff}$ values, resulting in an effective increase in the PPA, as well as the damping parameter. X-ray magnetic circular dichroism (XMCD) has also been performed on a series of V-doped films over a range of V concentrations. Magnetic tunnel junctions were fabricated to study device properties of the V-capped and V-doped films. The mechanisms for increasing TMR in these types of pMTJ's will be discussed.

This work is supported by the U.S. Department of Defense DARPA-MTO STT-RAM Universal Memory contract, and Grandis Inc., Milpitas, CA.

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11:00am **MI+TF-ThM10 Magnetic Properties of $Fe_xNi_{1-x}Fe$/Co Bilayers**, ***F.A. Perez***, *D. Lederman*, West Virginia University

11:20am **MI+TF-ThM11 Electrical Properties of $Ni.Fe_2O_3$ and $NiO.Fe_{1.925}Sm_{0.075}O_3$ Thin Films**, ***K.B. Karuppanan***, University of Texas at El Paso, *M. Garimalla,* IIT Madras, India, *C.V. Ramana*, University of Texas at El Paso

Nickel ferrite is one of the most versatile and technologically important ferrite materials because of its high Curie temperature, high saturation magnetization, low conductivity and thus lower eddy current losses, high electrochemical stability, catalytic behavior. The focus of the present work was to grow $Ni.Fe_2O_3$ and $NiO.Fe_{1.925}Sm_{0.075}O_3$ thin films by RF magnetron sputtering and study their structural and electrical properties. $Ni.Fe_2O_3$ and $NiO.Fe_{1.925}Sm_{0.075}O_3$ films were grown by sputtering the bulk $NiO.Fe_2O_3$ and $NiO.Fe_{1.925}Sm_{0.075}O_3$ targets prepared by solid state chemical reaction. The results indicate that the as-grown films were amorphous. Samples annealed at 1073 K were crystalline. DC electrical conductivity measurements performed in the temperature range 60-300 K indicate the insulating behavior of the materials. The room-temperature conductivity of the $NiO.Fe_{1.925}Sm_{0-075}O_3$ film is less than that of pure Ni ferrite film. Analysis of the conductivity indicates that the small polaron and variable-range-hopping (VRH) mechanisms are operative in 180–300 K and 60–180 K temperature regions, respectively. Frequency variation of the electrical resistivity measurements in the range 1 kHz - 13 MHz indicate that the resistivity decreases with increasing frequency. The mean relaxation time and spreading factor values were found to be larger for the $NiO.Fe_{1.925}Sm_{0-075}O_3$ film which could be due to the fact that larger Sm^{3+} ion leads to increased bond distance.

11:40am **MI+TF-ThM12 Structural, Transport and Magnetic Properties of $SrSn_{0.95}Fe_{0.05}O_3$ Thin Films**, ***G. Prathiba***, IIT Madras, India, *S. Venkatesh,* Tata Institute of Fundamental Research (TIFR), India, *N. Harish Kumar*, IIT Madras, India

Transparent magnetic semiconductors are potential materials for multifunctional magneto-opto-electronic devices. Wide band gap oxides are the best candidates for transparent semiconductors. Following the prediction of Dietl et al.,[1] on possible ferromagnetic ordering in wide band gap semiconductors doped with magnetic elements, the focus was on oxide dilute magnetic semiconductors. $SrSnO_3$ is a wide band gap material with a direct band gap of 4.27 eV. At room temperature it crystallizes in perovskite orthorhombic structure. The electrical resistivity of $SrSnO_3$ on forming solid solution with $SrFeO_3$ decreases. $SrSn_{0.95}Fe_{0.05}O_3$ thin films were prepared by RF magnetron sputtering on oxidized silicon (100) substrates at room temperature. The films were annealed at 1073 K for two hours. The as deposited films were found to be amorphous whereas the annealed films were polycrystalline in nature. The surface morphology of the films studied using Atomic Force Microscopy (AFM) showed low roughness value (Root mean square value of surface roughness – 2.02 nm). The resistivity of the film was measured using two probe method in the temperature range 200 to 300 K. The variation of resistivity with temperature exhibits semiconducting behaviour. Using Arrhenius plot [$\rho = \rho_o \exp(E/kT)$] the activation energy was found to be 0.39 eV. The magnetic measurements done using Superconducting Quantum Interference Device (SQUID) magnetometer showed ferromagnetic ordering below 20 K.

Reference:

[1]T. Dietl, H. Ohno, F. Matsukura, J. Cibert and D. Ferrand, *Science*, 287 (2000) 1018

Spectroscopic Ellipsometry Focus Topic
Room: Cochiti - Session EL+AS+EM+MS+TF-ThA

Spectroscopic Ellipsometry
Moderator: A.M. Creatore, Eindhoven University of Technology, the Netherlands

2:00pm **EL+AS+EM+MS+TF-ThA1 Developments in Spectroscopic Ellipsometry for Characterization of Organic and Inorganic Surfaces, Interfaces and Complex Layered Materials**, ***M. Schubert***, University of Nebraska - Lincoln **INVITED**

In this paper we will review new developments in Spectroscopic Ellipsometry for characterization of organic and inorganic surfaces, interfaces and complex layered materials. Ellipsometry has matured over the past two decades with instrumentation and methodology capable of addressing today's and tomorrow's challenges in materials characterization and metrology. Ellipsometry measures the general state of polarization of light reflected or transmitted from samples. Owing to its nondestructive and generally applicable concept of investigating light emerging from specimens under investigations, and owing to its extreme accuracy and precision, ellipsometry has paved the way for almost all our modern technologies, continues to enable next-generation devices in electronics and optoelectronics, and emerges into fields of chemical, biochemical and biological platform technologies. Originating from the identification that the information carried upon the polarization within a light beam emerging from surfaces is extremely sensitive to mono and submonolayer characteristics, ellipsometry started decades ago pioneering development of microprocessors and electronic devices, which still today are based on planar thin film technology. Without ellipsometry, today's computation and information technology would be still in its infancy. In this paper, emerging developments and applications for metrology of optical and electrical properties of semiconductors and nanostructures by Terahertz Magnetooptic generalized ellipsometry, also referred to as the Optical Hall effect, will be highlighted. Examples will include state-of-the-art nitride semiconductor device structures and epitaxial graphene, candidates for tomorrow's next-generation devices. Likewise, new approaches for characterizing precise structural, magnetic and optical properties of three-dimensional nanostructure hybrid materials will be discussed. Examples will describe how ellipsometry characterization enables understanding and tailoring of electromagnetic properties of materials created by human intelligence, rather than by nature. New horizons are being explored currently by combining ellipsometry with independent surface sensitive techniques, such as acoustic Quartz-Crystal microbalance techniques. Combinations allow for identification of new information not accessible otherwise. Examples include observation of in-situ formation of self-assembled monolayers, protein adsorption onto sensitized surfaces, and formation of micelle-assisted bilayer configurations. Prospects, challenges and future developments will be reviewed from today's perspective.

2:40pm **EL+AS+EM+MS+TF-ThA3 Characterizing the Adsorption – Desorption Behavior of Organic Molecules Within Thin Mesoporous Carbon Composite Films using Spectroscopic Ellipsometry**, ***B.D. Vogt***, *L.Y. Song, M.Z. Dai*, Arizona State University

Porous carbon materials are commonly utilized as adsorbants (i.e. activated carbon) and as catalyst supports. Direct templated synthetic routes to form ordered mesoporous carbons have recently been developed. By utilizing these concepts, mesoporous carbon composite films containing metal oxides can be synthesized. As a wide range of metal oxides can be utilized, these materials could be utilized in chemical sensing applications or as catalysts in fuel cell membranes. For both of these applications, the porous material will be exposed to organic vapors (such as ethanol in fuel cells). The condensation and evaporation of organic vapors from these materials is therefore an important consideration for their ultimate utilization in these applications. In-situ spectroscopic ellipsometry measurements of the mesoporous films exposed to controlled vapor pressures of organic vapors such as toluene, hexane and ethanol are utilized to understand the adsorption-desorption behavior of these films. Activated desorption of all three compounds is observed for pure carbon films, but addition of a small fraction of metal oxide enables the organics to be desorbed for the porous framework. These adsorption-desorption isotherms can also be utilized to estimate the pore size distribution and porosity of these films.

3:00pm **EL+AS+EM+MS+TF-ThA4 Mueller-Matrix Ellipsometry Studies of Chirality in Chitin-Based Structures and Thin Films of $Al_{1-x}In_xN$**, ***K. Järrendahl***, *H. Arwin, R. Magnusson, P. Sandström, C.-L. Hsiao, J. Landin, S. Valyukh, J. Birch*, Linköping University, Sweden

A limited number of natural structures are known to reflect light that has circular or near circular polarization. This is for instance, the case for some scarab beetles were it is suggested that the polarization is caused by chiral structures in the form of helicoids in the cuticles . In this study, Mueller-matrix spectroscopic ellipsometry is applied in the spectral range of 250 to 1000 nm to investigate optical response and structures of the cuticle of various scarab beetles of the Cetoniinae subfamily. We will present our measurements showing how the polarization changes with wavelength as well as incidence angle and specify the conditions for when the reflected light is circularly left- or right-polarized. In most cases the reflected light is left-polarized as described by negative values of the M41 Mueller matrix element. For *Cetonia aurata*, a green beetle with metallic appearance, this is clearly seen in a rather narrow spectral range (470-550 nm). For other beetles (*Potosia cuprea* and *Licola lugubris*) similar polarization behavior is observed but the polarization features occur in a broader spectral region. We will show that there are even beetles (e.g. *Plusiotis argentiola*) reflecting both left- ($M41 < 0$) and right-polarized light ($M41 > 0$) in different parts of the spectral region. The Mueller data, including observations of the degree of polarization, are used to obtain structural and optical parameters from model calculations.

Our attempts to fabricate artificial structures with similar polarization properties will also be presented. $Al_{1-x}In_xN$ thin films were grown on sapphire substrates by magnetron sputtering of indium and aluminum in a nitride atmosphere. Utilization of different seed layers and a substrate rotation gave chiral structures constituted by layers with a compositional gradient. Mueller-matrix results from these structures will be compared with the results from the natural structures. The Mueller data is also in this case very rich on information. In the initial steps to model these samples a similar approach as for the natural structures has been employed. Similarities and differences of the natural and artificial polarization response will be discussed in detail.

3:40pm **EL+AS+EM+MS+TF-ThA6 Mueller Polarimetry as a Tool for the Evaluation of the Diffraction Grating Profile Asymmetry**, ***T. Novikova***, *P. Bulkin,* LPICM, CNRS, Ecole Polytechnique, France, *V. Popov,* Moscow State University, Russia, *A. De Martino*, LPICM, CNRS, Ecole Polytechnique, France

Mueller polarimetry in conical diffraction has proved to be a powerful optical technique for the metrological characterization of diffraction gratings. It was already shown that the shape of grating profile can be successfully reconstructed via appropriate optical modeling using full Mueller matrix measurements [1]. We also demonstrated that this approach can be of particular interest in microelectronics technology for the detection of overlay errors, which frequently result from the alignment deficiencies in lithography [2]. In some cases the asymmetrical distortion of grating profile can be induced by the etch process, or even be intentional, like in blazed gratings fabrication. For these applications a technique that allows for fast non-contact evaluation of the profile asymmetry may be of great value.

We studied the Mueller matrix spectra of symmetrical [3] and asymmetrical photoresist diffraction gratings on chromium using MM16 spectroscopic polarimeter, commercially produced by Horiba Jobin-Yvon, in the most general geometry of conical diffraction. At this configuration the 0th order cross-polarization complex reflection coefficients are antisymmetrical ($r^0_{sp} = -r^0_{ps}$) , provided that the grating is composed of only reciprocal materials and is invariant under the rotation by 180° about the normal incidence [4]. It leads to the following relations between the elements of 2x2 off-diagonal blocks of Mueller matrix: $M_{ij} = \pm M_{ji}$.

The lack of rotational symmetry violates the electromagnetic reciprocity theorem for the 0th-order diffraction on the asymmetrical gratings and, consequently, breaks the symmetry of the off-diagonal blocks of Mueller matrix ($|M_{ij}|$ is not equal to $|M_{ji}|$). This property of Mueller matrix of asymmetrical gratings was experimentally observed and numerically modeled at any illumination condition with exception of planar and pure conical mounting. We showed that the non-reciprocity in diffraction gratings can be used for the unambiguous detection of the grating profile asymmetry. The optimal choice of measurement configuration, i.e. azimuthal and polar angles considerably increases the sensitivity of the above mentioned technique.

References:

[1] T. Novikova, A. De Martino, S. Ben Hatit, and B. Drévillon, Appl. Opt. **45**, 3688 (2006).

[2] T. Novikova, A. De Martino, R. Ossikovski and B. Drévillon, *Europ. Phys. J. Appl. Phys.* **31,** 63 (2005).

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4:00pm **EL+AS+EM+MS+TF-ThA7 Monitoring Ultra-Thin Organic Film Growth, *In-Situ*, with Combined Quartz Crystal Microbalance and Spectroscopic Ellipsometry**, ***K.B. Rodenhausen***, *B.A. Duensing, A.K. Pannier, M. Schubert,* University of Nebraska-Lincoln*, M. Solinsky,* The Procter & Gamble Company*, T.E. Tiwald*, J. A. Woollam Co., Inc.

We report a combinatorial approach to study ultra-thin organic films. This novel technique consists of *in-situ* spectroscopic ellipsometry and quartz crystal microbalance methods. In contrast to the quartz crystal microbalance, which is sensitive to the total mass attached to the surface, including the trapped solvent, spectroscopic ellipsometry only measures the amount of adsorbent on the surface. We also introduce a new "virtual separation approach" ($2\pi nd/\lambda \ll 1$) of analysis for the ellipsometry measurements. By using these two techniques in tandem, we are able to determine the thickness and solvent fraction of viscoelastic thin films.

We investigate cetyltrimethylammonium bromide (CTAB) thin films deposited onto a gold-coated quartz crystal as a model system. CTAB grown from a 2.5 mM solution demonstrates several phases in porosity evolution, including a temporary hold in water fraction as the film is rinsed off the substrate with water; these effects may be related to the structure of a CTAB bilayer.

In addition, a variety of self-assembled monolayers (SAMs) of alkanethiols on gold-coated quartz crystals are used as model biomaterials to determine the water fraction of an adsorbed prion layer. The porosity information distinguishes the proteins' conformation, dictated by the defined surface chemistries of the SAMs.

4:20pm **EL+AS+EM+MS+TF-ThA8 Ellipsometric Studies of Electronically Coupled PbSe and PbS Quantum Dot Thin Films**, ***S.G. Choi***, National Renewable Energy Laboratory*, O.E. Semonin,* University of Colorado*, J.M. Luther, M.C. Beard, A.G. Norman,* National Renewable Energy Laboratory*, Z. Lin,* Colorado School of Mines*, A. Franceschetti,* National Renewable Energy Laboratory*, M.T. Lusk,* Colorado School of Mines*, A.J. Nozik*, National Renewable Energy Laboratory

Discovery of multiple exciton generation from colloidal suspensions of semiconductor quantum dots (QDs) has generated growing interests in realization of high-efficiency QD-based solar cells. Among a number of semiconductor QDs explored up to date, lead chalcogenides such as PbSe and PbS have been of great interest as a result of their wide tuning range of bandgap energy, abundance of materials, and large exciton Bohr radius.

In this presentation, I discuss optical properties of electronically coupled PbSe and PbS QD thin films. A series of QD multilayer thin films were prepared by a layer-by-layer dip-coating method onto glass substrates. Diameter of the QDs varies from 3.2 to 7.2 nm and from 3.5 to 8.3 nm for PbSe and PbS, respectively. Room-temperature pseudo-optical functions of the samples were measured by a rotating compensator-type, variable-angle spectroscopic ellipsometer. Transmittance data were also acquired in a normal-incidence configuration.

First, I determined refractive index $N = n + ik$ of the QD films using the B-spline basis functions within the multilayer model (ambient/surface roughness/QD film/substrate). We use the N obtained as the input parameters for modeling the internal quantum efficiency of the QD-based solar cell devices. Then, I extracted dielectric function $\varepsilon = \varepsilon_1 + i\varepsilon_2$ for the ensemble of electronically coupled QDs using the Maxwell-Garnett effective medium approximations. The ε spectra show the first exciton peaks, and the E_1 and E_2 critical-point (CP) structures whose energies are higher than the corresponding bulk values probably due to the quantum confinement effects. This abstract is subject to government rights.

4:40pm **EL+AS+EM+MS+TF-ThA9 In-situ Temperature Measurements by Spectroscopic Ellipsometry: Application to a-Si based Thin Films**, ***D. Daineka***, LPICM, CNRS, Ecole Polytechnique, France*, V. Suendo,* Institut Teknologi Bandung, Indonesia*, P. Roca i Cabarrocas*, LPICM, CNRS, Ecole Polytechnique, France

Accurate measurement of the substrate temperature is of crucial importance in many semiconductor technologies such as plasma enhanced chemical vapor deposition (PECVD). Traditional tools, both thermocouples and pyrometers, are not always reliable for in situ measurements in vacuum when the substrate can be out of thermal equilibrium. On the other hand, non-contacting optical methods allow to determine the surface temperature with great accuracy, provided the temperature dependence of optical constants for the studied material is known. Since recently, spectroscopic ellipsometers are widely available and often installed on the research deposition systems, which provides an opportunity to use them for temperature monitoring. We have studied the optical functions of amorphous silicon based thin films with spectroscopic ellipsometry in the temperature range from 290 to 520 K. The experimental data were modeled using Tauc-Lorentz dispersion law for amorphous materials. We have found that the temperature coefficients of Tauc-Lorentz parameters, such as the optical gap, are rather close for a few different materials. That similarity suggests that these values can be used to determine the surface temperature for a broad range of amorphous silicon based materials with a good accuracy. Practical examples of using spectroscopic ellipsometry for temperature measurements in the low pressure PECVD environment are given.

5:00pm **EL+AS+EM+MS+TF-ThA10 Real Time Spectroscopic Ellipsometry Studies of Amorphous and Nanocrystalline $Si_{1-x}Ge_x$:H Thin Films for Microbolometer Applications**, ***D.B. Saint John***, *H.-B. Shin, M.-Y. Lee, E.C. Dickey, T.N. Jackson, N.J. Podraza*, Penn State University

Hydrogenated amorphous and nanocrystalline silicon (a/nc-Si:H), germanium (a/nc-Ge:H), and their alloys have been used and continue to be assessed for use in uncooled infrared microbolometer applications. These materials may be deposited as uniform layers using equipment common to the manufacturing of displays and photovoltaics and are thus more amenable to manufacturing considerations than the ion beam deposited vanadium oxide films used in most commercial microbolometers. Real optimization of material in the a/nc-$Si_{1-x}Ge_x$:H system for use in these devices requires a better understanding of the relationship between the key electrical properties of interest including resistivity (r), temperature coefficient of resistance (TCR), and the 1/f noise character as a function of the degree of order and composition of the films. $Si_{1-x}Ge_x$:H thin films were deposited using plasma enhanced chemical vapor deposition using SiH_4, GeH_4, and H_2 at variable H_2- dilution. These films have been monitored using in situ real time spectroscopic ellipsometry (RTSE) over a spectral range from 0.75 to 5.15 eV during deposition to detect changes in the film thickness and optical properties in the form of the complex dielectric function spectra ($e = e_1 + ie_2$) as a function of deposition time. From the RTSE measurements and analysis it is possible determine the structure of the material as amorphous, nanocrystalline, or mixed-phase and track the evolution of nanocrystallinity as a depth profile into the film. Ex situ Fourier transform infrared spectroscopic ellipsometry measurements over a spectral range from 0.05 to 0.75 eV were also performed to augment the complex dielectric function spectra and study absorption features relating to bonding. For electrical measurements, contacts were deposited in an isolated transfer length pattern for measurement of resistivity and TCR, while resistors with different volumes were made for volume normalization of the 1/f noise measurements. The TCR was measured from 20°C to 55°C. This study explores to correlations between the electrical and optical properties of a-$Si_{1-x}Ge_x$:H and nc-$Si_{1-x}Ge_x$:H as functions of film processing conditions, resultant composition, and order. a-$Si_{1-x}Ge_x$:H films were prepared as a function of germanium content and hydrogen dilution to identify the impact that germanium and improved order at higher hydrogen dilution conditions have on the electrical properties (r, TCR, 1/f noise). The impact on the electrical properties due to the incorporation of small fractions of nanocrystallites are explored using mixed-phase (a+nc)-Ge:H films with nanocrystallite profiles guided by depth profile studies.

5:20pm **EL+AS+EM+MS+TF-ThA11 Roll-to-Roll Fabrication of Thin Film Si:H Solar Cells: Real Time Monitoring and Post Deposition Mapping by Spectroscopic Ellipsometry**, ***L.R. Dahal***, *Z. Huang, D. Attygalle, M.N. Sestak, C. Salupo, S.X. Marsillac, R.W. Collins*, University of Toledo

Real time spectroscopic ellipsometry (RTSE) has been used to monitor the roll-to-roll deposition of thin film Si:H n-i-p solar cells on flexible plastic substrates coated with a Ag/ZnO back-reflector. In this process, the RTSE monitoring position is located directly above the ZnO sputtering target (i.e., at the closest target-substrate separation). RTSE data collection is initiated before the plasma is ignited so that ZnO nucleation can be observed. The film thickness increases with time until a steady state is reached, after which the bulk layer thickness at the monitoring point is constant with time. This occurs when the elapsed deposition time equals the time required for the moving substrate to travel from the leading edge of the deposition zone to the monitoring point. Although a constant substrate speed is selected such that the final film thickness is achieved in the time required to move through the entire deposition zone, this speed does not allow study of film growth that occurs after the substrate passes the monitoring point. To solve this problem, the substrate speed is reduced only in the early stage of growth such that the final film thickness of interest is reached at the monitoring point. In this way, RTSE can be used to analyze the entire layer on an initial length of the roll before the full length of the roll is processed. The thickness evolution of ZnO in the case of both normal and reduced

speeds shows good agreement with a simple inverse square variation of the deposition flux from the target to the flexible substrate.

After cell deposition, spectroscopic ellipsometry (SE) has also been applied for large area mapping of the completed 15 cm wide roll, at up to 1.5 m long sections at a time. Key information such as critical point, oscillator amplitudes, band gap energies, and widths have been extracted from which material density, composition, grain structure, disorder, and defect density can be determined. In this paper, optical mapping was applied for the intrinsic absorber layer in a full device a-Si:H solar cell structure. The results clearly show the degree to which thickness uniformity of the absorber layer depends on the gas flow and the electrode configuration. Also, by parameterizing the optical functions of the intrinsic absorber layer using single Lorentz oscillator modified by a low energy absorption cut-off, a map of its band gap and oscillator width can be deduced. Such an SE application is ideal for evaluation of uniformity in bulk thickness db, surface roughness thickness ds, index of refraction, and extinction coefficient (n, k); the critical parameters for fabricating uniform and high efficiency solar modules.

Graphene Focus Topic
Room: Brazos - Session GR+AS+TF+MI-ThA

Graphene: Surface Characterization
Moderator: P. Sutter, Brookhaven National Laboratory

2:00pm **GR+AS+TF+MI-ThA1 Scanning Tunneling Microscopy and Spectroscopy of Impurities on a Gated Graphene Device**, ***R.T. Decker***, *V.W. Brar, M.H. Solowan, Y.C. Wang, A. Zettl, M.F. Crommie*, University of California Berkeley **INVITED**

Understanding the scattering properties of electrons in graphene is important for controlling the behavior of different graphene nanostructure-based devices. Here we report a scanning tunneling microscopy (STM) and spectroscopy (STS) study of impurities on a single monolayer of graphene. In our experiments the graphene is placed on a layer of insulating SiO_2 that sits above a doped silicon back-gate electrode. We will discuss our observations of the electronic local density of states of impurities, as well as how these properties respond to electrical gating of the graphene monolayer with respect to the silicon back-gate electrode.

In particular, we will show that the combination of the back-gate voltage and the STM tip-gating effect allows the controlled ionization of the impurity when the resonance sweeps through the Fermi energy. The influence of this induced Coulomb potential on the electrons in graphene in the vicinity of the impurity will be discussed.

2:40pm **GR+AS+TF+MI-ThA3 Graphene Defect States in a Magnetic Field Studied by Scanning Tunneling Spectroscopy**, ***K.D. Kubista***, *D.L. Miller, M. Ruan, W.A. de Heer, P.N. First,* Georgia Institute of Technology, *G.M. Rutter, J.A. Stroscio*, National Institute of Standards and Technology

We present tunneling differential conductance (*dI/dV*) spectra and 2D conductance maps acquired over both positive and negative defects in magnetic fields up to 8 T. The measurements were performed on multilayer epitaxial graphene using scanning tunneling microscopy and spectroscopy at 4 K under ultrahigh vacuum conditions. Landau level drift states are found to follow the local potential (determined independently at near-zero magnetic field), but near a negatively-charged defect a bound (or quasibound) state originates from the $n = -1$ Landau Level. The defect state Stark shifts and finally ionizes under the influence of the STM tip electric field.

3:00pm **GR+AS+TF+MI-ThA4 Atomic-Scale Maps of Quantum Hall States in Epitaxial Graphene**, ***D.L. Miller***, *K.D. Kubista,* Georgia Institute of Technology, *G.M. Rutter,* National Institute of Standards and Technology, *M. Ruan, W.A. de Heer, P.N. First,* Georgia Institute of Technology, *J.A. Stroscio*, National Institute of Standards and Technology

When a perpendicular magnetic field is applied to a graphene sheet, the resulting eigenenergies (Landau Levels or LLs) have a nonlinear energy distribution that includes a four-fold degenerate zero-energy state (LL_0). Maps of the energy-resolved local density of states (LDOS) acquired via cryogenic scanning tunneling spectroscopy (STS) provide atomic-scale imaging of the LL spatial distribution. Focusing on LL_0, we use STS maps to image the *localized* and *extended* quantum Hall states. Unexpectedly, we find atomic-scale variations of the LDOS above a critical magnetic field. We attribute this to an energy gap in LL_0 and show how it depends on the local A-B lattice symmetry. The gap is observed only within patches of at least a few magnetic lengths in size, which forces the splitting to "turn off" below the critical field. This behavior implies a breaking of the local sublattice symmetry imposed by moiré layer stacking.

3:40pm **GR+AS+TF+MI-ThA6 Imperfect Graphene: Point Defects, Edges, Dislocations and Grain Boundaries**, ***O.V. Yazyev***, University of California, Berkeley **INVITED**

In two dimensions, properties of materials can be heavily affected by defects. In this talk, I will review our recent efforts directed towards understanding various types of structural irregularities in graphene.

Firstly, I will present the results of theoretical studies of the magnetism induced by point defects and edges in graphene and graphite. We show that in graphene single-atom defects such as vacancies and hydrogen chemisorption induce the spin-polarized defect states [1, 2]. The coupling between the magnetic moments is either ferromagnetic or antiferromagnetic, depending on whether the defects correspond to the same or to different sublattices of the graphene lattice, respectively. These results are able to clarify some experimental observations of high-temperature ferromagnetism in proton-irradiated graphite. Similarly, zigzag edges of graphene are predicted to induce spin-polarized edge states which can serve as a basis for novel spintronic devices. We address the question of the spin correlation length at finite temperatures in this one-dimensional magnetic system and establish the limitations of the proposed spintronic devices [3].

Then, I will talk about our latest results on dislocations and grain boundaries in graphene [4], topological defects which are still not well understood despites the growing number of experimental observations. We introduce a general approach for constructing dislocations in graphene characterized by arbitrary Burgers vectors as well as grain boundaries, covering the whole range of possible misorientation angles. By using ab initio calculations we investigate thermodynamic, electronic and transport properties of grain boundaries, finding energetically favorable large-angle symmetric configurations, strong tendency towards out-of-plane deformation in the small-angle regimes, pronounced effects on the electronic structure, and two distinct behaviors in the electronic transport [5] - either perfect reflection or high transparency for low-energy charge carriers depending on the grain boundary structure. Our results show that dislocations and grain boundaries are important intrinsic defects in graphene which may be used for engineering graphene-based functional devices.

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[2] O. V. Yazyev, Phys. Rev. Lett. 101, 037203 (2008).

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[4] O. V. Yazyev and S. G. Louie, arXiv:1004.2031 (2010).

[5] O. V. Yazyev and S. G. Louie, submitted.

4:20pm **GR+AS+TF+MI-ThA8 Spectroscopic Ellipsometry for Thickness Measurement and Optical Dispersion Modeling of CVD-Grown Graphene**, *F.J. Nelson, V.K. Kamineni,* ***A.C. Diebold***, The University at Albany-SUNY

Graphene has attracted much research over the past several years due to its electrical and mechanical properties. It is a prime candidate for electronic and optoelectronic devices, yet much of the research has utilized the exfoliation, or "scotch-tape" technique of sample preparation. More scalable growth methods have been investigated, such as the thermal decomposition of SiC, and the resulting graphene films have properties dependent on their fabrication parameters. One potentially scalable technique is that of hydrocarbon gas-based CVD onto metallic substrates. Here, we report on the ellipsometric measurement of Few-Layer-Graphene (FLG) grown on copper foils and subsequently transferred to a different substrate (i.e. glass). One of the challenges with development of a dispersion model for FLG is that the CVD graphene has many "grains" inside the measured area while previous reports of exfoliated graphene were done on single crystal samples. The work explores finding an average thickness, as well as the optical dispersion modeling, of the graphene layers on different substrates, such as SiO2/Si and glass slides.

Magnetic Interfaces and Nanostructures
Room: Southwest Exhibit Hall - Session MI-ThP

Magnetic Interfaces Poster Session

MI-ThP1 Investigations of Magnetic Overlayers at the Advanced Photon Source, ***G.D. Waddill***, Missouri University of Science and Technology, *S.W. Yu, M.T. Butterfield,* Lawrence Livermore National Laboratory, *T. Komesu,* Missouri University of Science and Technology, *J.G. Tobin*, Lawrence Livermore National Laboratory

Magnetic overlayers of Fe and Co have been investigated with X-ray Magnetic Circular Dichroism in X-ray Absorption Spectroscopy (XMCD-XAS) and Photoelectron Spectroscopy (PES), including Spin- Resolved Photoelectron Spectroscopy (SRPES), at Beamline 4 at the Advanced Photon Source (APS). Particular emphasis was placed upon the interrogation of the 2p levels of the Fe.

MI-ThP2 Magnetic Properties of Size-Selected Fe (FeAu) Nanoparticles, ***K. Paredis***, University of Central Florida

We report the magnetic properties of size-selected Fe and FeAu nanoparticles (NPs) supported on SiO2/Si(001). These microscopic properties are dominated by two key parameters: finite size effects and surface effects.

In order to systematically study size effects, we use the method of inverse micelle encapsulation (PS-P2VP diblock - cop ol ymers) for the growth of the nanoparticles. This approach results in Fe (and FeAu) NPs with a high homogeneity in size, shape and inter-particle distance. Following this method, the NP size can be tuned by changing the length of the polymer head (P2VP) while the interparticle distance can be modified by changing the length of the polymer tail (PS). Investigating these NPs in-situ (ultrahigh vacuum) after the removal of the encapsulating ligands by means of a variable temperature magneto-optical Kerr effect set-up enables the determination of: (i) the temperature dependen ce of the coercivity and remanence of the NPs, (ii) the blocking temperature for the ferromagnetic-superparamagnetic transition, and (iii) the direction of magnetization in anisotropic nanostructures . This new insight constitutes a step forward towards unrave l ling the influence of the NP geometrical structure (size and shape) on its magnetic properties. Additionally, by varying the interparticle distance we can probe the role played by particle-particle interactions in the collective magnetic behavior.

MI-ThP3 Fabrication of a Non Local Spin Logic Device with Exfoliated Graphene Channel, ***J.R. Abel***, *A. Matsubayashi, J.J. Garramone, V.P. LaBella*, University at Albany

The use of the electron spin has gained considerable attention lately as a possible substitute for charge-based electronics [1,2]. This poster will focus on the fabrication of a spin logic device that utilizes graphene as the spin transport channel since graphene has been shown to have a long spin lifetime at room temperature [3]. The device is prepared utilizing exfoliated graphene on SiO_2. The injection and readout contacts were fabricated with and without aluminum oxide as a tunnel barrier which was deposited using thermal evaporation of Al in ultra high vacuum (UHV) and then subsequent oxidation in O_2. Then Co/Au was deposited under high vacuum and 100-200-nm-wide contacts were pattered using e-beam lithography followed by a standard liftoff technique. Scanning electron microscopy and optical images will be presented of the fabrication process and the device. Non-local spin valve and Hanle measurements are being pursued to characterize the spin injection polarization and the spin relaxation in the graphene channel.

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MI-ThP4 Magnetic Properties of $Zn_{1-x}Mn_xO$ Thin Film Grown by Pulsed Laser Deposition, ***T.C. Wu***, *Y.C. Yeh, D.R. Liu,* National Applied Research Laboratories, Taiwan, *H.J. Lin, M.J. Huang*, National Synchrotron Radiation Research Center, Taiwan

In this paper, $Zn_{1-x}Mn_xO$ (x=0~0.1) thin films were grown on corning glass 、sapphire (0001) and silicon (100) substrates by pulsed laser deposition (PLD). Atomic force microscopy (AFM) and magnetic force microscopy (MFM) were used to characterize the surface properties of $Zn_{1-x}Mn_xO$ thin film, and the high-resolution x-ray diffraction (XRD) was used to measure the crystallographic structure of this film. Moreover, superconducting quantum interference device (SQUID) magnetometer was employed to investigate the magnetic moments. X-ray magnetic circular dichroism (XMCD) spectra of $Zn_{1-x}Mn_xO$ films were also measured to clarify their spin and orbital magnetic moment properties. Integrating above measurements, these results reveal that substrate plays an important role and oxygen is the key factor for magnetic properties of $Zn_{1-x}Mn_xO$ thin films.

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