Monday Morning, October 29, 2012

Actinides and Rare Earths Focus Topic Room: 6 - Session AC+MI+SS+TF-MoM

Electronic Structure and Spectroscopy of Actinides

Moderator: A.J. Nelson, Lawrence Livermore National Laboratory

9:00am AC+MI+SS+TF-MoM3 Strong Correlations and the Electronic Structure of the Actinide Dioxides, *R.L. Martin*, Los Alamos National Laboratory INVITED

The series of actinide dioxides (AnO2, An=Pa, ... Cm) are difficult challenges for electronic structure theory. The early members of the series are Mott insulators, the band gap corresponding to *f-f* transitions, while the later members, beginning with PuO2, are $O2p \rightarrow An5f$ charge transfer insulators. I will review recent experimental results (X-ray absorption, photoemission and optical band gaps) which now allow us to distinguish among several many-body approximations to their electronic structure, including the SIC, DFT+U, DMFT+U and hybrid DFT (HSE) approaches.

9:40am AC+MI+SS+TF-MoM5 Synchrotron Radiation Studies of Actinide Compounds, S.M. Butorin, Uppsala University, Sweden INVITED

Core-to-core resonant inelastic x-ray scattering (RIXS) and valence-to-core RIXS techniques are two complimentary ways for probing the electronic structure in actinide systems. Specific cuts of the core-to-core RIXS maps around $M\beta$ and $L\alpha$ lines of actinides represent remarkably improved high-resolution x-ray absorption spectra of actinide 3d and 2p edges, respectively, as a result of limited lifetime broadening of core holes present in shallower levels in the final state of the spectroscopic process. That allows for more detailed studies of unoccupied states and better oxidation states assignments. In turn, the valence-to-core RIXS spectra are only limited by the instrumental resolution and provide information about actinide chemical bonding and interactions between valence electrons.

A comparison of experimental data with results of model calculations shows that the resonant spectra of actinide systems recoded at the actinide M(3d) and O(5d) thresholds which probe the 5f states can be interpreted using the many-body theory, such as the Anderson impurity model, while the data obtained at the L3 threshold and representing the 6d states of actinides can be described within a single-particle approach, such as LDA+U (local density approximation with supplemented Coulomb interaction U) framework.

In course of discussion of the above statements, we present the RIXS data for a number of actinide systems with emphasis on the results contributing to understanding of the U-O and Pu-O phase diagrams, in particular data for UO2+x, U4O9, U3O8 and PuO2+x. The influence of the Coulomb interaction between 5f electrons on the electronic structure of actinides is also discussed.

10:40am AC+MI+SS+TF-MoM8 Quasiparticle Dynamics in Uranium Systems from Ultrafast Spectroscopies, *T. Durakiewicz*, Los Alamos National Laboratory

Every time we add a new dimension to an experimental method, we open a window to novel, unexpected and fascinating phenomena. Here we show the results of our focused effort of adding time-domain to the powerful experimental techniques of Angle Resolved Photoelectron Spectroscopy (ARPES) and reflectivity. The novel tools are applied to actinides and help us understand the details of the electronic structure of the correlated f-electron materials.

In the hidden order system URu_2Si_2 we investigate the massive renormalization of the Fermi surface at specific k values. The application of time-resolved ARPES allowed a direct measurement of the momentumresolved quasiparticle lifetime which was shown to increase by an order of magnitude at the hidden order transition. Time-resolved ARPES together with the ultrafast reflectivity results provided evidence for forming a multiple gap structure, including the hybridization gap, pseudogap and HO gap [1, 2].

Another actinide system of interest is a Mott insulator UO_2 , where we have investigated the complex dynamics of the Hubbard excitons. We have found that the dynamics can be divided into four distinct processes: instantaneous hop, picosecond lattice deformation, phonon emission and relaxation, and the slow relaxation related to the propagation of Hubbard excitons [3]. We have also obtained the first direct measurement of Hubbard gap in 5f system [4].

The novel femtosecond pump-probe methods provide unique information about the dynamics of 5f quasiparticles, and open novel possibilities in addressing the long-standing questions about the role of near-Fermi level band renormalization in establishing the physical properties of correlated materials.

References

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11:00am AC+MI+SS+TF-MoM9 Comparison of Spectroscopic Data with Cluster Calculations of Plutonium, Plutonium Dioxide and Uranium Dioxide, J.G. Tobin, S.W. Yu, B.W. Chung, Lawrence Livermore National Laboratory, M.V. Ryzhkov, Russian Academy of Science-Ekaterinburg, A. Mirmelstein, Russian Federation Nuclear Center-Snezhinsk

Using spectroscopic data produced in the experimental investigations of bulk systems, including X-Ray Absorption Spectroscopy (XAS), Photoelectron Spectroscopy (PES) and Bremstrahlung Isochromat Spectroscopy (BIS) [1-5], the theoretical results within for U0₂ [6], PuO₂ [6] and Pu [7] clusters have been evaluated. The calculations of the electronic structure of the clusters have been performed within the framework of the Relativistic Discrete-Variational Method (RDV). [6,7] The comparisons between the LLNL experimental data and the Russian calculations are quite favorable. The cluster calculations may represent a new and useful avenue to address unresolved questions within the field of actinide electron structure, particularly that of Pu. Observation of the changes in the Pu electronic structure as a function of size suggests interesting implications for bulk Pu electronic structure.

Acknowledgements

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Oxide Heterostructures-Interface Form & Function Focus Topic Room: 7 - Session OX+EM+MI+NS+TF-MoM

Structure–Property Relationships in Epitaxial Oxide Interfaces

Moderator: E.I. Altman, Yale University

8:20am OX+EM+MI+NS+TF-MoM1 Role of Dual-laser Ablation in Controlling Mn Oxide Precipitation during the Epitaxial Growth of Mn Doped ZnO Thin Films with Higher Doping Concentrations, D. Mukherjee, M. Hordagoda, R.H. Hyde, N. Bingham, H. Srikanth, P. Mukherjee, S. Witanachchi, University of South Florida

The low solubility of Mn (equilibrium limit of 13 %) and precipitation of Mn oxides at slightly higher Mn doping (> 4 %) have remained major obstacles in the growth of Mn doped ZnO (ZnO:Mn) thin films for potential spintronic applications. In this work, epitaxial ZnO:Mn thin films were deposited on c-cut Al₂O₃ (0001) substrates, with increasing Mn concentrations from 2 to 12 %, using the dual-laser ablation process. In this process, an excimer (KrF) laser and a CO₂ laser pulses are spatially and temporally overlapped onto the target surface. Initially the target is heated by the CO2 laser to produce a transient molten layer, from which the slightly time-delayed KrF laser initiates the ablation. Ablation for a momentary liquid target not only results in a drastic reduction of particulates in the deposited films but also overcomes the problem of non-congruent ablation of the ZnO:Mn target, leading to stoichiometric film deposition. Moreover, the optimum coupling of the laser energies produces an ablation plume that has a broader angular distribution, compared to the plume generated by KrF pulse alone, as observed from the intensified-charge-coupled-detector (ICCD) images of the ablated plumes. This allows the deposition of uniform films over larger area. Further, the higher ionization of the ablated species as seen in the optical emission spectra (OES) of the dual-laser ablated plumes leads to enhanced gas phase reaction and better film morphology and crystallinity. X-ray diffraction studies revealed that the dual-laser deposited ZnO:Mn films were single crystalline with no secondary phase formation even at 12 % doping while single-laser deposited ZnO:Mn films showed secondary Mn oxide phases. Room temperature magnetic measurements showed ferromagnetism (FM) with enhanced saturation magnetization (Ms) values from 1.3 emu/cm3 for 2 % ZnO:Mn films to 2.9 emu/cm³ for 12 % ZnO:Mn films. In- and out-of-plane magnetization revealed absence of magnetic anisotropy. Further, temperature dependent Hall measurements showed a strong correlation between the effective carrier densities and the observed FM. All these measurements suggested a carrier mediated mechanism of FM in ZnO:Mn thin films. Using both the experimental data and theoretical analysis the FM in less conducting ZnO:Mn films was described by a bound magnetic polaron model whereas that in highly conducting films was consistent with a carrier mediated interaction via RKKY exchange mechanism.

8:40am OX+EM+MI+NS+TF-MoM2 Structural Characterization of Heterojunction *n*-ZnO/*p*-NiO Thin Films Epitaxially Deposited on (0002)Al₂O₃ Substrates, *Y.H. Kwon*, Sungkyunkwan University, Republic of Korea, *J.H. Lee*, KAIST, Republic of Korea, *S.H. Chun*, Sungkyunkwan University, Republic of Korea, *J.Y. Lee*, KAIST, Republic of Korea, *H.K. Cho*, Sungkyunkwan University, Republic of Korea

Recently, oxide semiconductors with superior electical properties have been considered as candidates to replace Si based electronics. Furthermore, their thermally and chemically stable characteristic is preferable for devices. Especially, among a lot of oxides, ZnO based semiconductors have been extensively investigated to apply in wide application such as thin film transistor and light emitting diode. ZnO is an intrinsic *n*-type semiconductor which characteristic comes from Zn interstitials and O vacancies. And band-gap and exciton binding energy are 3.37 eV and 60 meV, respectively, which is suitable for optical application operating in ultra-violet region. Therefore, *p*-*n* homojunction diode structure combined with *n*-ZnO and *p*-ZnO having well matched interface had been studied by a lot of researchers.[1] However, it was not reliable since *p*-type ZnO synthesized by doping of group V elements is unstable and return to the *n*-type by self-compensation.[2]

Therefore, *p*-*n* heterojunction diode composed of *n*-ZnO and stable *p*-type oxide such as Cu₂O and NiO was alternatively studied.[3] Among the *p*-type oxides, NiO with wide direct band-gap (3.7 eV) have been expected to apply in optical applications. And conductivity of NiO could be significantly controlled by Li+ doping. Furthermore, according to T. Dutta et. al., (111) plane of NiO could well matched with (0002) of ZnO by domain match epitaxy.[4]

In this study, heterojunction diode structure was fabricated with *n*-type ZnO and *p*-type NiO on [0002] oriented Al₂O₃ substrates. RF magnetron sputtering method was used for deposition of NiO and ZnO films. After the deposition of NiO films at 400°C in O₂ atmosphere, ZnO films were grown at 600°C and in Ar and O₂, mixed gas atmosphere. XRD result showed the NiO films were fabricated with high crystallinity and preferred orientation of [111]_{NiO}. And sixfold symmetry of (100)_{NiO} plane obtained by phi-scan indicates that the NiO films were bi-epitaxially grown on Al₂O₃ substrates. In addition, electrical properties of NiO showed relatively low resistivity (1.648 Ω cm) and high mobility (14.52 cm²/Vs) due to Li⁺ doping. Sixfold symmetry of (1-102)_{ZnO} observed at phi-scan result indicates that ZnO films were also epitaxially grown on [111] oriented NiO films.

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9:00am OX+EM+MI+NS+TF-MoM3 Manipulating the Electrostatic Boundary Conditions of Polar Interfaces, Y. Hikita, SLAC National Accelerator Laboratory INVITED

Transition metal oxides (TMO) offer various functionalities ranging from electronic devices to environmental catalysts [1, 2]. Often, the central part of such devices is the interface between different materials. In order to improve their device performance, control of charge transport across these interfaces is essential. Originally developed in semiconductor heterostructures, interface band alignment control is based on the interface electrostatic boundary conditions and is one of the most fundamental methods to tune the carrier transport across interfaces [3]. Given their strongly ionic nature and their accessibility to multiple valence states, the TMO interface should be more suitable than covalent semiconductors for manipulating interface band alignments. Here we focus on epitaxial metalsemiconductor Schottky interfaces between perovskite oxides to demonstrate the effectiveness of this technique. I will present two SrTiO₃ based perovskite Schottky junctions in which the interface energy barriers were modulated by interface dipoles controlled on the atomic scale [4]. Further, I will present the application of this technique in the form of an alloxide hot electron transistor [5].

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11:20am OX+EM+MI+NS+TF-MoM10 Strain-induced Oxygen Vacancy Ordering at SrTiO₃/La_{0.5}Sr_{0.5}CoO₃ Interfaces, and its Impact on Magnetic "Dead" Layers, *S. Bose, M. Sharma, M. Torija,* University of Minnesota, *J. Gazquez, M. Varela,* Oak Ridge National Laboratory, *J. Schmitt, C. He,* University of Minnesota, *S. El-Khatib,* American University of Sharjah, United Arab Emirates, *M. Laver, J. Borchers,* NIST Center for Neutron Research, *C. Leighton,* University of Minnesota

The remarkable functionality and epitaxial compatibility of complex oxides provides many opportunities for new physics and applications in oxide heterostructures. Perovskite cobaltites provide an excellent example, being of interest for solid oxide fuel cells, oxygen separation membranes, catalysis, ferroelectric RAM, resistive switching memory, and oxide spintronics. However, the same delicate balance between phases that provides this diverse functionality also leads to a serious problem - the difficulty of maintaining desired properties close to the interface with other oxides. Although this problem is widespread, manifests itself in several ways, and could present a significant roadblock to the development of heterostructured devices for oxide electronics, there is no consensus as to its origin. In our work, using SrTiO3(001)/La1-xSrxCoO3 as a model system, we have combined epitaxial growth via high pressure oxygen sputtering [1] with high resolution x-ray diffraction, atomic resolution scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS), and detailed magnetic, transport, and neutron scattering measurements to determine the fundamental origin of the deterioration in interfacial transport and magnetism [2,3]. The effect is found to be due to nanoscopic magnetic phase separation in the nearinterface region driven by a significant depletion in interfacial hole doping due to accumulation of O vacancies. This occurs due to a novel mechanism for accommodation of lattice mismatch with the substrate based on formation and long-range ordering of O vacancies [4]. This fundamental

link between strain state and O vacancy formation and ordering is explored in detail in this presentation. We demonstrate that the O vacancy density, depth profile, and ordering vector can all be controlled via strain, leading to a potential mechanism to substantially improve interfacial properties.

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11:40am OX+EM+MI+NS+TF-MoM11 Fabrication and Characterization of Titanium Oxide Films with Tunable Stiffness, K. Gotlib-Vainshtein, O. Girshevitz, C.N. Sukenik, Bar Ilan University, Israel, D. Barlam, Ben Gurion University, Israel, E. Kalfon-Cohen, S.R. Cohen, Weizmann Institute of Science, Israel

The design of surfaces with controlled stiffness is attractive for a variety of applications ranging from controlling cell growth to mechanical and electrical engineering design. Here, the creation of layered composites with tunable surface stiffness has been achieved by coating a soft PDMS polymer with a stiff film of amorphous titanium oxide with thickness varying from 2 to 50 nm. The oxide layer is smooth (6 nm rms roughness at $2 \mu m^2$ image size), and crack-free. Air plasma treatment was used to form a silica surface layer on the soft polymer base to promote of adhesion of the titania overlayer. To gain insight into the mechanics of the layered structure, nanomechanical quantification has been performed using different experimental approaches, as well as modeling studies. The surface mechanical properties of the samples have been probed using both instrumented nanoindentation and atomic force microscopy—based nanomechanical characterization. These results have been compared to finite element analysis (FEA) simulations.

By fitting the FEA simulations with experimental curves it is shown that the hard titania film and softer PDMS substrate individually maintain their characteristic elastic moduli, while the stiffness of the vertical nanocomposite can be controllably modified by changing the thickness of the stiff layer. Liquid phase deposition of the oxide allows control of its thickness at the nm level. During an indentation cycle, the stiff layer transmits the stress to the underlying PDMS base by deformation of its overall shape, but only negligible compression of the film thickness.

This synthetic approach can be quite versatile, and can, in principle, be extended to different oxides and a wide range of thicknesses. It allows control of surface properties while maintaining bulk material properties. This exploratory work is a first step towards defining the range of surface stiffnesses that can be achieved in this way, as well as developing general methodologies for their characterization.

Monday Afternoon, October 29, 2012

Actinides and Rare Earths Focus Topic Room: 6 - Session AC+TF+SS+MI-MoA

Actinides and Rare Earths: Thin Films and Surface Science

Moderator: R.K. Schulze, Los Alamos National Laboratory

AC+TF+SS+MI-MoA1 Rare Earth 4f Hybridization in 2:00pm Gallium Nitride, J.W. McClory, S.R. McHale, Air Force Institute of Technology, L. Wang, W.N. Mei, University of Nebraska-Lincoln, J.C. Petrosky, Air Force Institute of Technology, J. Wu, R. Palai, University of Puerto Rico - San Juan, Ya.B. Losovyj, Louisiana State University, P.A. Dowben, University of Nebraska-Lincoln INVITED The location of the Gd, Er and Yb 4f states within the GaN valence band has been explored both experimentally and theoretically. The 4d - 4fphotoemission resonances for various rare earth doped GaN thin films (RE = Gd, Er, Yb) provide an accurate depiction of the occupied 4f state placement within the GaN valence band. The resonant photoemission show that the major Er and Gd rare earth 4f weight is at about 5-6 eV below the valence band maximum, similar to the 4f weights in the valence band of many other rare earth doped semiconductors. For Yb, there is very little resonant enhancement of the valence band of Yb doped GaN, consistent with a largely $4f^{4-d}$ occupancy. The placement of the rare earth 4f levels is in qualitative agreement with theoretical expectations.

2:40pm AC+TF+SS+MI-MoA3 Revisiting the Yb Electronic Structure with Low-Energy Photoemission Spetroscopy, F. Offi, CNISM and Univ. Roma Tre, Italy, P. Vilmercati, L. Petaccia, S. Gorovikov, ELETTRA Sincrotrone Trieste, Italy, A. Ruocco, CNISM and Univ. Roma Tre, Italy, M.I. Trioni, CNR-ISTM, Milano, Italy, A. Rizzo, CNISM and Univ. Roma Tre, Italy, A. Goldoni, ELETTRA Sincrotrone Trieste, Italy, G. Stefani, CNISM and Univ. Roma Tre, Italy, G. Panaccione, CNR-IOM, Basovizza-Trieste, Italy, S. Iacobucci, CNI-IFN, Rome, Italy

The peculiar electronic structure of rare-earth elements and compounds is mostly defined by the partially filled 4f band. Of particular interest is the investigation of the valence states, which is linked to the degree of hybridization of f electrons with delocalized s-d bands. In the simple case of Yb, the 4f states are fully occupied with a Fermi level of 6s character and a 2+ valency. However, the occupation of the Yb valence band has been the subject of several investigations over the years, intended in particular to separate the contribution of 5d states. Early experimental photoelectron emission (PES) spectra at very low excitation energy (hv < 10 eV) have reported a spectral modulation in the region close to the Fermi level that was attributed to the emission from a 5d band. The poor energy resolution did not allow however a detailed investigation of such spectral features. In recent years this low energy photoemission spectroscopy (LEPES) encountered a renewed interest, under the stimulus of the extremely high energy resolution obtainable with laser excited LEPES and given the expectation of a large increase of the bulk sensitivity at these low energies. W e monitored the 4f spectral intensity in polycrystalline Yb films in the LEPES regime (between 5.5 and 21 eV photon energy, with experiments at the BaDELPH beamline of the ELETTRA synchrotron radiation facility), observing a moderate increase of the electron attenuation length and, thus, a moderate increase of the information depth when we reach the lowest energies. By lowering the photon energy below about 11 eV a prominent peak at the Fermi level is observed. The analysis of its intensity variation versus photon energy and the comparison of the experimental spectra with ab initio density of states (DOS) calculations allow to attribute this structure to a p band crossing the Fermi level, enhanced at selected photon energies due to the influence of the empty DOS, probably amplified by a photoionization cross section effect and by the general increase of the photoelectron yield at low photon energy. In this respect LEPES may thus be considered as a probe of the joint DOS.

3:00pm AC+TF+SS+MI-MoA4 Erbium Rare Earth Thin Film Hydride Stress Studies as a Function of Processing Techniques, J.L. Provo, J.L. Provo Consulting

An important part of understanding the behavior of rare earth, Group 3A and 4A thin film hydrides is the determination of indirect effects such as stress in the film lattice which can lead to film flaking. In this study, special vacuum sample containers were prepared to observe and record basal-plane film stress levels, and film flaking (optical observations).

The special vacuum sample containers contained erbium deuteride (${\rm ErD}_2)$ and erbium tritide (${\rm ErT}_2$) films on AT and BT quartz resonator substrates with chromium underlays in pairs prepared by air-exposure, (in-situ)

evaporate-load and reactive evaporation hydriding techniques. The erbium deuteride samples were prepared as controls for aging studies. All samples were processed with PVD Electron Beam deposition techniques, hydriding techniques mentioned above and a 450°C temperature bakeout and exhaust in consideration of the $\alpha \rightarrow \beta$ crystal phase transformation in crystalline quartz at 573°C.

Samples for the measurement of initial film deposition stress as a function of hydride processing and for the determination of stress produced in ErT_2 films due to the generation of helium-3 with time (i.e., tritium decay) were designed to utilize the double- resonator technique developed by EerNisse(1). Measurements of mass change and induced film stress were determined by frequency measurement changes obtained with a precision frequency counter, data being taken from the output of a one transistor Colpitts type driving oscillator circuit in which the crystal is an integral part.

A summary of initial film deposition stress (tensile) and film aging accumulative stress (compressive) for the erbium films from the different deposition and hydriding techniques is given. Reactively evaporated erbium occluder films were seen to have an initial film deposition tensile stress approximately 5 times less than (in-situ) evaporate-load films and 11 times less than air-exposed loaded films. Acculumative aging compressive stress for erbium occluder films were shown to be more variable but data indicate that reactively evaporated film aging stress is less than that of (in-situ) evaporate-load and air –exposed tritided films.

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3:40pm AC+TF+SS+MI-MoA6 Splat Cooling Technique Contributing to Understanding of Uranium Systems, L. Havela, Charles University, Czech Republic, A. Gonçalves, J.-C. Waerenbogh, L. Pereira, ITN Sacavém, Portugal, I. Tkach, Charles University, Czech Republic, N.-T. Kim-Ngan, Pedagogical University Cracow, Poland, T.B. Scott, University of Bristol, UK

The splat cooling technique is one of the methods of ultrafast cooling of a melt, particularly suitable for small amounts of material. In particular cases it can help to overcome constraints imposed by thermodynamics. One of them was the issue of magnetic properties of non-stoichiometric Laves phase UFe2. This compound has a ferromagnetic ground state (with both U and Fe magnetic moments). An excess of U, achieved by quenching, led to the decrease of $T_{\rm C}$ from 162 K for pure compound to 112 K for UFe_{1.7} [1]. Quenching was, however, unable to provide Fe-rich material, with expected increase of T_c. Using splat cooling of a series of materials with various offstoichiometry from UFe2 to UFe6 we found that the cubic Laves phase structure (with sum-micron grains) can absorb excessive Fe up to the stoichiometry UFe_{2,3}. Additional excess leds to the segregation of α -Fe [2]. The increase of TC up to 230-240 K was the impact on magnetic properties. The spontaneous magnetization also increases from 1.0 $\mu_B/f.u.$ in UFe₂ to 1.9 $\mu_B/f.u.$ in UFe_{2.3}. ⁵⁷Fe Mössbauer spectroscopy reveals that the excessive Fe atoms enter the U sublattice and develop higher magnetic moments (approx. 1.0 µ_B/Fe).

Applying the splat cooling technique on pure and doped U metal had the aim to stabilize the high temperature *bcc* phase (γ -U) to low temperatures, to be able to establish its basic electronic properties. In particular, changes in magnetic characteristics and electronic specific heat can be expected due to the modest volume expansion comparing to orthorhombic α -U. We found that splat cooling reduces the necessary concentration of dopants and U with 12 at.% Mo has no traces of α -U. The Sommerfeld coefficient $\gamma = 19$ mJ/mol K^2 estimated for pure $\gamma\text{-}U$ is enhanced comparing to 11 mJ/mol K^2 for pure U splat, which is close to values given in literature [3] for the U metal. The splats exhibit a superconducting ground state with T_c ranging from 1.24 K for pure U to 2.11 K for 15 % Mo. The γ-U superconductivity is characterized by a large critical field exceeding 6 T and a sharp λ -type anomaly in specific heat $C_p(T)$ with the size corresponding to the BCS theory. The superconductivity of a pure U splat, which contains only traces of γ -U, has much lower critical field (0.33 T) and the weak anomaly in $C_{\rm p}(T)$ does not convince about the bulk character of superconductivity.

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4:00pm AC+TF+SS+MI-MoA7 Investigation of Rare Earth Doped Lithium Tetraborate Glasses with XAFS and Emission and Excitation Spectroscopy, *T.D. Kelly, J.W. McClory, D.A. Buchanan, A.T. Brant, J.C. Petrosky,* Air Force Institute of Technology, *Ya.B. Losovyj,* Louisiana State University, *V.T. Adamiv, Ya.V. Burak,* Institute of Physical Optics, *P.A. Dowben,* University of Nebraska-Lincoln

The local structure of rare earth doped lithium tetraborate ($Li_2B_4O_7$) glasses has been studied by extended x ray absorption fine structure (EXAFS) at the rare earth L shells and by optical emission and excitation spectroscopies. The samples investigated were 1% rare earth doped by weight with Gd and Nd. The EXAFS signal was recorded in fluorescence mode with the energies calibrated for Nd L1 and L3 edges and Gd L3 edge. X rays were applied to the samples to activate emission and excitation centers in the glasses. The spectra were analyzed to determine rare earth occupation sites in the lithium tetraborate crystal structure and the emission and excitation lines due to rare earth doping.

4:40pm AC+TF+SS+MI-MoA9 Eu-implanted p-type GaN: Charge-Driven Luminescence Hysteresis and Identification of a Possible Charge-State-Alternation Resonance of the Mg Acceptor, K.P. O'Donnell, P.R. Edwards, R.W. Martin, Strathclyde University, Scotland, UK, K. Lorenz, E. Alves, V. Darakchieva, ITN Sacavém, Portugal, M. Bockowski, Unipress, Poland

Europium-doped p-type GaN shows spectral switching and luminescence hysteresis when samples are temperature-cycled between room temperature and 20 K (K.P. O'Donnell et al, Late News paper at ICPS2012, Zurich). An explanation of this unusual behaviour may be found in the charge-state dependence of the local structure of the Mg acceptor in GaN, recently modelled by J.L. Lyons et al., (Phys. Rev. Lett. 108, 156403 (2012)). Eu ions, sensitive to their local environment, may act as 'spectators' of the charge-induced local distortions. The dominant impurity-induced luminescence spectrum at RT (hereafter, Eu0) switches completely to another spectrum (Eu1) when samples are cooled below 25 K. Upon subsequent warming of the sample, Eu1 fades with increasing temperature, as expected, but Eu0 does not reappear until the temperature exceeds 150 K; its recovery is complete only above 210 K. The noted temperature extremes correspond to hole localisation (carrier freeze-out) and delocalisation, respectively. Here, we extend Lyons' model to consider the possibility of observing the resonance in which the acceptor alternates rapidly between neutral and negative charge states, leading to a spatial oscillation of the associated defect between Eu0 and Eu1 forms, and describe the possible spectral identification of this resonance.

Oxide Heterostructures-Interface Form & Function Focus Topic

Room: 7 - Session OX+SS+TF+MI-MoA

Chemistry of Oxide Surfaces and Interfaces

Moderator: M. Engelhard, EMSL, Environmental Molecular Sciences Laboratory

2:00pm OX+SS+TF+MI-MoA1 Investigation of Al₂O₃ Nanostructure Surfaces Using Charge Optimized Many Body Potentials, *D.E. Yilmaz*, *T. Liang*, *S.B. Sinnott*, *S.R. Phillpot*, University of Florida

Aluminum oxide nanostructures have drawn attention due to their Interesting physical and optical properties. In particular, photoluminescence peaks for these systems are attributed to oxygen vacancies and surface effects. Here, we apply third-generation Charge Optimized Many Body (COMB) potentials for the Al-A₁₂O₃ system to investigate the properties of Al₂O₃ nanoparticle surfaces. In particular, the elastic properties and local atomistic strain distribution of nanoparticles with a range of sizes are determined, and the corresponding vibrational spectra are determined. The effect of oxygen vacancies and adsorbed surface atoms on the local strain and vibrational spectra are also determined. This work is supported by the National Science Foundation (DMR-1005779).

2:20pm OX+SS+TF+MI-MoA2 Manipulating Ferroelectric Surfaces for Direct NO_x Decomposition, M.W. Herdiech, A. Kakekkhani, S. Ismail-Beigi, E.I. Altman, Yale University

Current technology for removing nitrogen oxides from engine exhausts relies on nearly stoichiometric air to fuel ratios. Under these conditions, the concentrations of CO and unburned hydrocarbons in the exhaust stream are high enough to efficiently remove adsorbed oxygen from the platinum based catalysts in catalytic converters, ensuring that the catalysts do not become saturated with adsorbed oxygen. Direct catalytic decomposition of NO_x to N₂ and O₂ in the presence of excess O₂ would eliminate the need for

reducing species in automobile engine exhaust streams, allowing these engines to be run more efficiently. We have been investigating the potential of ferroelectric supports to modify the behavior of supported layers to enable direct NO_x decomposition. Our approach involves first principles density functional theory and surface science techniques. Using both approaches we have investigated the interactions of N, O, and NO with bare ferroelectric lead titanate surfaces and surfaces modified to expose catalytic layers, in particular Ru oxides. Theory indicates that the behavior of the PbTiO₃ surface towards these species is sensitive to the polarization direction and termination of the ferroelectric and that stable RuO2terminated surfaces can be created by manipulating the termination of the substrate. Experiments take advantage of plasma sources that allow the behavior of O and N atoms to be studied individually and expitaxial growth to manipulate the termination of the ferroelectric support. Favored reaction pathways are assessed using theory and temperature programmed desorption and related mass spectrometry methods.

2:40pm OX+SS+TF+MI-MoA3 Catalyst Synthesis by Atomic Layer Deposition, P.C. Stair, Northwestern University & Argonne National Laboratory INVITED

Atomic Layer Deposition (ALD) has enormous potential for the synthesis of advanced heterogeneous catalysts with control of composition and structure at the atomic scale. The ability of ALD to produce conformal oxide coatings on porous, high-surface area materials can provide completely new types of catalyst supports. At the same time ALD can achieve highly uniform catalytically active metal and oxide phases with (sub-) nanometer dimensions.

Vanadium oxide species supported on high surface area oxides are among the most important catalytic materials for the selective, oxidative conversion of hydrocarbons to useful chemicals. In our laboratory ALD has been used to synthesize both the catalytic vanadium oxide and the supporting oxide on both high surface powders and anodic aluminum oxide (AAO) nanoliths. These materials have been characterized by SEM, XRF, ICP, UV-Vis absorption spectroscopy, Raman spectroscopy and evaluated for the oxidative dehydrogenation (ODH) of cyclohexane.

More recently we have studied the synthesis of supported metal particles and developed what we call "ABC-type" ALD in which metal nanoparticles and support materials are grown sequentially in each ALD cycle. This method makes possible the synthesis exceptionally small particles, ca. 0.5 nm. Using additional ALD support layers at the conclusion of the growth, the metal particles can be stabilized against sintering while still remaining active at high temperatures and reaction conditions. Moreover, the catalysts resist coke formation which is a leading cause of catalyst deactivation. These properties are imparted as a result of anchoring step and edge atom sites while leaving facet sites open for catalysis.

3:40pm OX+SS+TF+MI-MoA6 Energy Alignment at Organic/Oxide Interfaces: The Influence of Adsorption Geometry and Chemical Bond on Interface Dipole, S. Rangan, C. Ruggieri, S. Coh, R.A. Bartynski, K. Chitre, E. Galoppini, Rutgers University

The lack of control of the energy alignment at the interface between an organic layer and an oxide substrate remains a limitation to the performance of promising technologies such as dye sensitized solar cells, organic light emitting diodes or organic thin film transistors. The energy alignment depends not only on the choice of the starting materials, but also on more subtle parameters such as oxide surface termination or defects, and molecular layer preparation mode.

In an effort to disentangle the different aspect of the interface of an organic/oxide system, we have studied simultaneously the adsorption geometry and the energy alignment of the Zn(II) tetraphenylporphyrin (ZnTPP) molecule on the TiO2(110) and ZnO(11-20) surfaces. Two approaches have been pursued: 1) in-situ evaporation of the ZnTPP on a clean oxide surface prepared in ultra-high vacuum resulting in weakly bound multilayers or monolayers 2) ex-situ sensitization in a solution of ZnTPP derivative, modified with COOH anchoring group for chemisorption at the oxide surface.

Scanning tunnel microscopy has been used to characterize the clean oxides and the ZnTPP adsorption modes. X-ray photoemission, ultra-violet photoemission and inverse photoemission spectroscopies have allowed the exploration of both occupied and unoccupied states of the electronic structure, resulting in the full characterization of the energy alignment at the surface as a function of the molecular overlayer thickness. The electronic transport gap, obtained from the latter experimental techniques has also been compared to the optical gap obtained from reflection electron energy loss spectroscopy, thus allowing the characterization of bound excitonic states.

The effect of the ZnTPP/oxide interface preparation, as well as the effect of the oxide substrate on the energy alignment will be presented. The

discussion will be extended to metallic substrates such as $\mathrm{Ag}(100)$ and $\mathrm{Au}(111)\,\mathrm{surfaces}$

4:00pm OX+SS+TF+MI-MoA7 Energy-Level Alignment at Organic/Oxide Interfaces, M.T. Greiner, Z.-H. Lu, University of Toronto, Canada INVITED

Oxide/organic interfaces play an important role in many organic electronic device designs. Oxides are frequently used as buffer layers to tune the energy-level alignment between electrodes and organic semiconducting layers, and thus allow for efficient hole/electron injection. As per the 'integer charge-transfer' (ICT) model, energy-level alignment at electrode/organic interfaces is governed by the electrode's Fermi level and the organic molecule's oxidation/reduction potential. While the ICT model was originally proposed for organic/organic interfaces, it also applies to a broad range of transition metal oxides. In this presentation we will discuss the energy-level alignment (ELA) of several organic semiconductors with transition-metal oxides. We will show that ELA is primarily governed by an oxide's work function, and that ELA is relatively insensitive to oxide electronic structure. As transition metal oxides can exhibit a wide range of work functions (~ 2 - 7 eV), and can possess a wide range of electronic properties (p-type to n-type) they are very versatile materials for use in organic electronics. We will their properties-such as work function and electronic structure-can best be utilized for use as buffer layers in organic light-emitting diodes and organic photovoltaics.

4:40pm OX+SS+TF+MI-MoA9 Variable Kinetic Energy XPS of the Buried P3HT/ITO Interface, *M.T. Brumbach*, Sandia National Laboratoria *I.C. Waisik* National Institute of Standards and Tachnology

Laboratories, J.C. Woicik, National Institute of Standards and Technology The characterization of buried interfaces is difficult and often has to be performed by post-processing methods where the interface is revealed, disturbed, and possibly altered by environmental exposure. Variable kinetic energy X-ray photoelectron spectroscopy (VKE-XPS) offers the ability to tune the depth of analysis while the use of hard X-rays allows for a deeper analysis. The combination of variable energy hard X-rays for XPS (HAXPES) allows for systematic evaluation through a buried interfacial region. An important inorganic/organic interface for use in organic photovoltaic devices is the poly(3-hexylthiophene) (P3HT) interface with indium tin oxide (ITO). In this work P3HT/ITO buried interfaces were examined using X-ray energies from 2.2-3.9 keV. The ITO surface was additionally prepared using different pretreatment conditions. The P3HT film protected the ITO surface from adventitious adsorbents and allowed for sensitivity to the buried ITO surface. Robust peak fitting parameters were obtained to model the O 1s and In 3d lineshapes. The deconvolution of these lineshapes allowed for the clear identification of a surface layer on the ITO which is oxidized to a greater extent than the underlying bulk ITO. The surface oxide layer, composed of indium oxide and indium hydroxide, is deficient of oxygen vacancies and would therefore be expected to act as an insulating barrier on the ITO surface. Peak fitting conditions allowed for an estimation of the thickness of this insulating layer. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

5:00pm OX+SS+TF+MI-MoA10 Organic Molecules Adsorbed on the ZnO(10-10) Surface: An Infrared Reflection Absorption Spectroscopy Study, *M. Buchholz*, Karlsruhe Institute of Technology, Germany, *H. Noei*, *Y. Wang*, Ruhr University Bochum, Germany, *A. Nefedov, Ch. Wöll*, Karlsruhe Institute of Technology, Germany

Except for gold, every metal forms an oxide on its surface when exposed to the ambient atmosphere. The understanding of chemical processes taking place on metal oxide surfaces are thus of crucial importance. One of the most important oxides is ZnO. As a result of its semiconducting and optical properties, this material is used in many applications such as gas sensors, thin film solar cells, as well as in photocatalysis and photooxidation[1]. The important surfaces of ZnO are the polar Zn- or O-terminated ZnO(0001) and ZnO(000-1) as well as the mixed-terminated ZnO(10-10) surface. The latter is the dominating surface for ZnO powder particles and energetically most favorable.

Here we report on the adsorption of formic acid and maleic anhydride (MA) molecules on the mixed-terminated ZnO(10-10) surface. Formic acid is a good model molecule for understanding the anchoring of carboxylic dye molecules in dye-sensitized solar cells. The choice of MA is motivated by the importance of the industrial process where MA is hydrogenated using Cu/ZnO catalysts. The identification of the reaction mechanism requires the identification of intermediates using IR-spectroscopy[2].

In last decades numerous IR investigations of oxide powders have been reported. An unambiguous assignment of the features present in the complex powder IR spectra, however, is only possible on the basis of reference data recorded for well-defined systems, e.g. surfaces of single crystals with defined orientation. Unfortunately, Infrared Reflection Absorption Spectroscopy(IRRAS) studies of molecular adsorbates on oxide single crystals, and, inparticular on ZnO, are extremely scarce due to the fact that the sensitivity of IRRAS to adsorbate vibrations is two orders of magnitude lower for oxides than for metals. Whereas in case of TiO2 recently with improved experimental setups adsorbate vibrations have been observed for a number of cases[3], to our knowledge molecular vibrations on clean ZnO single crystal surfaces have not yet been reported. With our novel UHV-IRRAS setup[4] high-quality IR spectra of different molecular adsorbates on ZnO(10-10) could be recorded in a routine fashion. In this presentation the obtained results will be presented and discussed.

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5:20pm OX+SS+TF+MI-MoA11 In Situ Interface Analysis of Self-Assembled Monolayers on Metal Surfaces at High Water Activities by Means of a PM-IRRAS/QCM-Setup, I. Giner, M. Maxisch, G. Grundmeier, University of Paderborn, Germany

Aluminum and its alloys are widely used as engineering material and in a wide range of applications ranging from the aviation industry to the automotive and construction industries. As almost all engineering metals, aluminum under ambient conditions is covered by a native oxide film which alters significantly its surface physical and chemical properties. For corrosion protection and adhesion promotion, oxide covered aluminum surfaces are coated with organic films. Ultra-thin films or even monomolecular layers of organic acids like self-assembled monolayers (SAMs) of organophosphonic and organocarboxylic acids have been investigated as new advanced interfacial layers for aluminum alloys.1 However, the stability of the self-assembled monolayers under environmental conditions is an aspect for technical applications. Different studies concerning to the stability and structure of the self-assembly monolayers under high humidity's conditions have been performed.2 These studies revealed that the organic film decreased the amount of interfacial water layer but cannot prevent the water diffusion through the monolayer.3 The aim of the present work is to establish an in-situ setup combining quartz crystal microbalance (QCM) and PM-IRRAS to study the chemistry of passive films and adsorbed organic monolayers at high humidity. The metal coated quartz was used as the reflecting substrate for the PM-IRRAS measurement. Thereby, the structure of the monolayer, the amount of adsorbed water and the chemical state of the surface layer in the presence of an adsorbed water layer could be analysed in-situ. The surface hydroxyl density prior to organic molecule adsorption was adjusted by means of low temperature Ar- and H2O- plasma treatments. Adsorption studies of H2O on nonadecanoic carboxylic acid (NDA) monolayer modified surfaces in comparison to bare oxide covered aluminum surfaces showed, that the NDA monolayer leads to a reduced amount of adsorbed water based on the inability of water to form hydrogen bonds to the low energy aliphatic surface chemistry. Moreover the kinetics of chemisorption of water indicated by the oxyhydroxide peak growth at SAM/metal interfaces could be significantly inhibited. Furthermore, it is noticeable that interfacial carboxylate group coordinatively bound the oxide as well as the orientation of the NDA monolayer is not affected by the adsorption of several monolayers water. Bibliography 1. Thissen, P et al. Langmuir 2010, 26, (1), 156-164 2. Thissen, P et al. Surface & Coatings Technology 2010, 204 (21-22), 3578-3584. 3. Maxisch, M et al. Langmuir 2011,27 (10), 6042-6048

Tuesday Morning, October 30, 2012

Graphene and Related Materials Focus Topic Room: 13 - Session GR+AS+EM+MI+MN-TuM

Optical, Magnetic, Mechanical and Thermal Properties Moderator: K.I. Bolotin, Vanderbilt University

8:00am GR+AS+EM+MI+MN-TuM1 Characterization of Magnetically Tunable Iron Nanorod Coated Graphene Nanoplatelets, S.D. Johnson, M.H. Gowda, S.-F. Cheng, N.Y. Garces, B. Feigelson, F.J. Kub, C.R. Eddy, Jr., U.S. Naval Research Laboratory

Composites made from iron coated graphene nanoplatelets (GNPs) show promise for applications such as, magnetic switches, electromagnetic interference shielding, and electromagnetic waveguides due to the large conductivity of GNPs combined with the magnetism of iron. Additionally, this composite can be easily formed into millimeter thick sheets making it a promising composite for other applications.

We report a novel method to synthesize iron oxide compound onto GNP using microwave hydrothermal synthesis at 60° C and reaction times between 10 and 120 minutes. Scanning electron microscopy imaging reveals iron oxide nanorods approximately 100 nm long adhered to the GNPs for reaction times as short as 10 minutes. X-ray photoemission spectroscopy reveals that the iron/carbon ratio remains constant across these reaction times. The resistivity of the composite increases with reaction time from 0.2 to 0.6 ohm-cm. Saturation magnetization and coercive field values follow a decreasing trend with increasing reaction time. From 10 to 120 minutes saturation magnetization decreases by 70% from 170 emu/g and coercive field decreases by 40% from 52 Oe. Remnant magnetization of around 0.7 memu/g remains constant throughout. We also report the temperature-dependent magnetic response of the compound across the Morin transition, which for submicron particles of α -Fe₂O₃ is near 250 K.

Preliminary results suggest that while the nanorod size and quantity remains constant with reaction time, the resistive and magnetic properties change. This may suggest that we are tuning the magnetism of the system by changing the iron structure between the ferromagnetic γ -Fe₂O₃ and the antiferromagnetic α -Fe₂O₃.

8:20am GR+AS+EM+MI+MN-TuM2 Dynamical Origin of Blue Photoluminescence from Graphene Oxide, A.L. Exarhos, M.E. Turk, P.M. Vora, J.M. Kikkawa, University of Pennsylvania

The tunable broadband emission from graphene oxide (GO) has sparked significant interest in research regarding its potential for band gap engineering. Here, we use polarization sensitive time-resolved optical spectroscopy to study the spectral diffusion and sub-picosecond dynamics of the excited carriers in GO and photo-exposed GO, where photo-exposure has been demonstrated to constitute a reducing condition. In steady state measurements, a significant blueshifting of the photoluminescence (PL) is observed with photo-exposure. This blueshift correlates with a marked difference in the temporal behavior of the PL from GO and photo-exposed GO. The PL spectra are very similar at short delay times, but an increased non-radiative recombination rate in the exposed GO leads to a decreased lifetime in the material. Utilizing in-plane polarization memory measurements, we examine the electron-hole polarization in these systems which can probe excitonic effects and help to provide a better understanding of the role of the sp² graphene lattice in GO and exposed GO. We further discuss the relevance of our data to the origins of PL in these systems.

A.L.E. gratefully acknowledges the support of NSF DMR-0907226. M.E.T., P.M.V., and the construction of a Kerr gate system are supported by the Department of Energy Office of Basic Energy Sciences Award DE-SC0002158.

8:40am **GR+AS+EM+MI+MN-TuM3** Spin-Transport and Magnetism in Graphene, *R. Kawakami*, University of California, Riverside **INVITED** Graphene is an attractive material for spintronics due to its high mobility and the low intrinsic spin-orbit and hyperfine coupling, which should lead to excellent spin transport properties. In 2007, graphene became the first material to exhibit gate tunable spin transport and spin precession at room temperature. However, the spin injection efficiency was low and the spin lifetime was much shorter than predicted theoretically. In this talk, I will report on our progress in this area. The low spin injection efficiency into graphene is due to the conductivity mismatch between the ferromagnetic metal (Co) spin injector and the single layer graphene (SLG). To alleviate this problem and enhance the spin injection efficiency, we developed atomically smooth MgO tunnel barriers by utilizing a TiO₂ seed layer. With tunneling contacts, the non-local spin signal is found to be as high as 130 ohms at room temperature, with a spin injection efficiency of 30%. In addition to improving the spin injection efficiency, the tunneling contacts were found to improve the spin lifetime as well. This indicates that the short spin lifetimes reported before are due to the contact-induced spin relaxation from the ferromagnetic electrodes. Using tunneling contacts, we investigate spin relaxation in single layer graphene (SLG) and bilayer graphene (BLG). At low temperatures, contrasting behaviors of gate voltage dependence of the spin lifetime are observed between SLG and BLG, which suggest different mechanisms for spin relaxation in SLG and BLG. A final topic of interest is magnetism and the formation of magnetic moments in graphene. While there is substantial theoretical work on magnetic moments generated by hydrogen adatoms and lattice vacancies, the experimental situation is less clear. We have developed a new method for detecting magnetic moment formation based on scattering of pure spin currents in graphene spin valves. We will report the progress on our efforts to identify magnetism with this approach.

10:40am **GR+AS+EM+MI+MN-TuM9** A "How To" for Magnetic Carbon, *H. Ohldag*, SLAC National Accelerator Laboratory, *E. Arenholz, T. Tyliszczak,* Lawrence Berkeley National Laboratory, *D. Spemann, R. Hoehne, P. Esquinazi, M. Ungureneau, T. Butz,* University of Leipzig, Germany

While conventional wisdom says that magnetic materials have to contain some metallic atoms, the confirmation of intrinsic magnetic order in pure metal free carbon represents an ultimate and general scientific breakthrough because of the fundamental importance of carbon as an elemental building block of organic as well as inorganic matter. The common controversy raised across all disciplines is whether the magnetism of carbon is intrinsic or induced by other elements. We address this controversy by providing clear experimental evidence that metal free carbon can be ferromagnetic at room temperature using dichroism x-ray absorption spectro-microscopy. For this purpose we acquired soft x-ray microscopy images of magnetic structures on a thin carbon film that have been produced by irradiation with a focused 2.25MeV proton beam. Our element specific magnetic probe shows no indication of magnetically ordered Fe, Co or Ni impurities in these samples. In a second step we investigate the particular electronic states that are involved in carbon magnetism and find that the carbon pstates as well as C-H bonds show a magnetic moment, indicating that hydrogenation plays a crucial role in developing the ferromagnetic order. Our surface sensitive approach reveals that the magnetism at the surface of the irradiated graphite samples is much larger than in the bulk of the sample. We observe a surface magnetic moment similar to what is typically present in classical ferromagnetic 3d transition metals.

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11:00am **GR+AS+EM+MI+MN-TuM10** From Graphene to Amorphous Carbon by Sublimation and Condensation, *B. Steele*, *R. Perriot*, *V. Zhakhovsky*, *I.I. Oleynik*, University of South Florida

The mechanisms of the non-equilibrium melting process of graphene and the structure of the liquid phase of carbon was studied by molecular dynamics (MD). Graphene undergoes a non-equilibrium melting process at high temperature and low pressure as the carbon chains are formed out of the graphene sheet, thus making up a transient liquid phase of carbon. As the chains expand the material sublimates to a low dense gas of carbon chains. Under higher pressure the gas phase will condense to an intermediate porous phase of carbon with a significant sp² fraction of atoms, followed by the liquid phase, and finally an amorphous phase. Mechanisms of melting of graphene, including formation of topological and Stone Wales (SW) defects in two and three dimensions will be discussed.

Tuesday Afternoon, October 30, 2012

Magnetic Interfaces and Nanostructures Room: 6 - Session MI+EN+BI-TuA

Fundamental Problems in Magnetism

Moderator: G.J. Szulczewski, The University of Alabama

2:00pm MI+EN+BI-TuA1 Spintronics - Implications for Energy, Information and Medical Technologies, S.D. Bader, Argonne National INVITED Laboratory and Northwestern University Spintronics encompasses the ever-evolving field of magnetic electronics.[1,2] Fields such as spintronics are hold the potential to extend the information technology revolution as the semiconductor road map reaches its end . A major issue with present day electronics is in its demand for increased power. Spintronics offers the possibility to communicate via pure spin currents as opposed to electric charge currents. The talk provides a brief perspective of recent developments to switch magnetic moments by spin-polarized currents, electric fields and photonic fields. Developments in the field of spintronics continue to be strongly dependent on the exploration and discovery of novel nanostructured materials and configurations. An array of exotic transport effects dependent on the interplay between spin and charge currents have been explored theoretically and experimentally in recent years. The talk highlights select promising areas for future investigation, and, features recent work at Argonne, [3,4] including, most strikingly, in the realm of medical applications. [5]

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Samuel D. Bader, Materials Science Division and Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois 60439, and Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208 USA

2:40pm MI+EN+BI-TuA3 Multiscale Modeling for Spintronics, K.A. Mewes, T. Mewes, W.H. Butler, University of Alabama INVITED The next generation of spintronic devices relies strongly on the development of new materials with high spin polarization, optimized intrinsic damping and tunable magnetic anisotropy. Therefore technological progress in this area depends heavily on the successful search for new materials as well as on a deeper understanding of the fundamental mechanisms of the spin polarization, the damping and the magnetic anisotropy. My talk will focus on different aspects of materials with high spin polarization, low intrinsic relaxation rate and perpendicular anisotropy. Our results are based on first principles calculations in combination with a non-orthogonal tight-binding model to predict those material properties for complex materials which can be used for example in new spin based memory devices or logic devices. Future progress in spintronics not only requires a better understanding of the underlying physical principles but also hinges strongly on the development of theoretical models capable of describing the expected performance of realistic device structures. As an example I will discuss the challenges in the Spin Transfer Torque Random Access Memory. This memory is dense, fast and nonvolatile and has the capability of a universal memory possibly even replacing today's Dynamic Random Access Memory (DRAM).

4:00pm MI+EN+BI-TuA7 Anomalous Magneto Transport in Amorphous TbFeCo Film with Perpendicular Magnetic Anisotropy, N. Anuniwat, M. Ding, J. Poon, S.A. Wolf, J.W. Lu, University of Virginia

TbFeCo has attracted some interests because of its high perpendicular anisotropy and tunable magnetic properties for nanomagnetic and spintronics application. Due to the fact that electronic device is getting smaller, fundamental understanding of size and geometry dependent is crucial. In this study, we report a strong size dependence of the coercive field in 15 - 100nm thick Tb30Fe63.5Co6.5 films with MgO capping. Magneto Optical Kerr effect (MOKE) and Vibrating Sample Magnetometer are performed on unpatterned films. The films exhibited strong PMA characteristics. The films were then fabricated into Hall bars with 10 μ m, 50 μ m, 100 μ m and 500 μ m in width. From anomalous Hall effect (AHE), HC was determined for these patterned films. We observed coercivity enhancement as the width of the hall bar decreases (up to 200% at room temperature). The temperature dependent of the coercivity is also studied. There exhibits the local minimum as the temperature change from 50 - 300K. The correlation between HCmin and dimensions of the hall bar are discussed. The magnetic domain structures and surface morphology analysis were performed using magnetic force microscopy and atomic force microscopy respectively. The variation in domain sizes , structures for different hall bars as well as possible origins of the coercivity enhancement are also discussed.

4:20pm MI+EN+BI-TuA8 Magnetic Properties of Fe Clusters: A DFT+U vs Nano DFT+DMFT Analysis, A.K. Kabir, V. Turkowski, T.S. Rahman, University of Central Florida

We use our recently proposed combined density-functional-theory/dynamical-mean-field-theory (DFT + DMFT) approach for molecules and nanosystems [1] to study the magnetic properties of Fe clusters consisting of 15, 17 and 19 atoms. This method has several advantages compared with the widely-used DFT + U approach for systems with localized electron states, the most important of which is that it takes into account dynamical correlation effects. These effects are especially important in the case when the kinetic (hopping) and the local Coulomb repulsion energies have the same order of magnitude. In particular, we study the size-dependence of the magnetic properties of the clusters by using the nanoDMFT code developed in our group using the iterated-perturbation theory approximation in the impurity solver. We find that the DFT+DMFT approach yields much better agreement for the magnetization with experimental data as compared to DFT and DFT+U methods, both of which generally overestimate the magnetization.

Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354

1. V. Turkowski, A. Kabir, N. Nayyar and T.S. Rahman J. Phys.: Condens. Matter 22, 462202 (2010) and J. Chem. Phys. 136, 114108 (2012)

4:40pm MI+EN+BI-TuA9 Rationally-designed Iron Oxide Nanostructures for Bioimaging, Y. Bao, The University of Alabama INVITED

Iron oxide nanoparticles have been extensively studied in targeted delivery, localized therapy, and as contrast agents for magnetic resonance imaging (MRI). In fact, sugar coated iron oxide NPs have been clinically used as the liver/spleen-specific contrast agents in MRI, indicating the biocompatibility and potential of iron oxide nanoparticles in nanomedicine. This presentation will discuss how rationally designed iron oxide nanoparticles can achieve highly effective MRI contrast agents. The talk will primarily focus on the shape control of iron oxide nanoparticles and the surface functionalization. The formation and magnetic properties of various shaped-iron oxides (e.g., cubes, nanoworms, nanoplates, and nanowires) will be elaborated. In particular, ultrathin iron oxide nanowires will be discussed in details, such as synthesis, property, and their potential as MRI contrast agents.

5:40pm MI+EN+BI-TuA12 3D Vector Magnetometry of Thin-Films using Generalized Magneto-Optical Ellipsometry (GME), J.A. Arregi, J.B. González-Díaz, O. Idigoras, A. Berger, CIC nanoGUNE Consolider, Spain

Generalized Magneto-Optical Ellipsometry (GME) has emerged in the last decade as a methodology to characterize magnetic materials with a high degree of precision, by means of utilizing the magneto-optical Kerr effect [1]. Compared to other magneto-optical characterization methods based on the same effect, GME has two key advantages: it can measure both the optical and magneto-optical constants, and it allows full vector magnetometry, all with one simple experimental set-up. The technique has been successfully employed in the study of diverse magnetization reversal processes, for the purpose of identifying spin-polarized electronic states in multiferroic materials [2], as well as for the measurement of the magnetization orientation using 2D vector magnetometry [3].

Even if some works have suggested the possibility to perform quantitative 3D vector magnetometry using the GME technique [4], actual measurements have not been demonstrated so far. Here, we extract the field dependent evolution of the three magnetization components during the reversal process. In order to do so, we exploit the different symmetries of the longitudinal, transverse and polar Kerr effect around different polarizer/analyzer crossing points, which allows us to separate the information of each of the magnetically induced contributions to the non-diagonal reflection matrix elements. By combining the presence of in-plane uniaxial anisotropy as well as out-of-plane applied magnetic fields in our

Co and Co-alloy based thin films, we manage to monitor the evolution of the full magnetization vector as a function of the field.

In addition to this full vector magnetometry capability, we have recently improved this technique to enhance measurement reliability [5] and we also extended its capabilities to characterize materials that are magneto-optically active and optically anisotropic at the same time [6].

References:

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[2] M. Bastjan, S. G. Singer, G. Neuber et al., Phys. Rev. B 77, 193105 (2008)

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[6] J. B. González-Díaz, J. A. Arregi, E. Bergaretxe, M. J. Fertin, O. Idigoras, and A. Berger, submitted to *Appl. Phys. Lett.*

Scanning Probe Microscopy Focus Topic Room: 16 - Session SP+AS+BI+ET+MI+NS-TuA

Advances in Scanning Probe Imaging

Moderator: S. Allen, The University of Nottingham, UK, Z. Gai, Oak Ridge National Laboratory

2:00pm SP+AS+BI+ET+MI+NS-TuA1 Molecules Investigated with Atomic Resolution using Scanning Probe Microscopy with Functionalized Tips, L. Gross, F. Mohn, N. Moll, G. Meyer, IBM Research - Zurich, Switzerland INVITED

Single organic molecules were investigated using scanning tunnelling microscopy (STM), noncontact atomic force microscopy (NC-AFM), and Kelvin probe force microscopy (KPFM). With all of these techniques submolecular resolution was obtained due to tip functionalization by atomic manipulation. The techniques yield complementary information regarding the molecular structural and electronic properties.

Using NC-AFM with CO terminated tips, atomic resolution on molecules has been demonstrated and the contrast mechanism was assigned to the Pauli repulsion [1]. On the other hand, by using STM the molecular frontier orbitals, i.e., the highest occupied and the lowest unoccupied molecular orbitals (HOMO and LUMO), were mapped [2]. Using a CO terminated tip for orbital imaging with the STM, the resolution can be increased and the images correspond to the gradient of the molecular orbitals due to the *p*-wave character of the tip states [3]. Finally, KPFM reveals information about the distribution of charges within molecules by measuring the *z*-component of the electrostatic field above the molecule, as demonstrated on the hydrogen tautomerization switch naphthalocyanine [4].

References :

[1] L. Gross et al. Science 325, 1110 (2009).

[2] J. Repp et al. Phys. Rev. Lett. 94, 026803 (2005).

[3] L. Gross et al. Phys. Rev. Lett. 107, 086101 (2011).

[4] F. Mohn et al. Nature Nanotechnol. 7, 227 (2012).

2:40pm SP+AS+BI+ET+MI+NS-TuA3 Functional Imaging of Jahn-Teller Dynamics at the Single-molecule Scale, J. Lee, S.M. Perdue, A. Rodriguez Perez, P.Z. El-Khoury, V.A. Apkarian, University of California, Irvine

Taking advantage of both elastic and inelastic tunneling processes of a molecule isolated at the double-barrier tunneling junction of a scanning tunneling microscope, both static and dynamic parts of the Hamiltonian can be visualized with submolecular resolution. This is illustrated by imaging Jahn-Teller (JT) driven vibronic dynamics within Zn-etioporphyrin (ZnEtio), in its various reduced forms, in what may be regarded as nature's choice of a molecule as a controllable current switch. Unique interpretations are afforded through simultaneously recorded functional images, such as maps of: a) energy resolved differential current, b) spectrally resolved electroluminescence, c) conduction bistability, d) reduction/oxidation potentials (maps of charging and discharging). We focus on the radical anion, ZnEtio, which is reduced by injecting an electron to a single ZnEtio molecule adsorbed on a thin aluminum oxide film grown on NiAl(110). In contrast with the neutral, the saddle-shaped radical anion lies flat on the surface of the oxide. The discharge map directly shows that the excess electron is localized in the ²p_x orbital of the entire porphyrin macrocycle, as a result of the JT active rectangular (B1g) distortion of the molecule. The static JT potential leads to conduction bistability, with reversed switching polarity depending on whether tunneling electrons are injected in the occupied ${}^{2}p_{x}$ orbital or the diamond (B_{2g}) coordinate which serves as a transition state that connects the p_{x} and p_{y} orbitals at the two B_{1g} minima. In addition to the JT switching, the dynamic JT states are directly imaged through electroluminescence spectra, induced by injection of a second electron in the anion. The spectra consist of a continuum due to radiative ionization of the dianion, and sharp Fano resonances of the vibronic progression of the JT active modes. A detailed analysis of the spectra yields the vibronic couplings and the wavefunctions. Vibronic structure is inherent in STM topographic images, and has hitherto not been fully recognized.

3:00pm SP+AS+BI+ET+MI+NS-TuA4 Atomic and Chemical Resolution of Heterogeneous 1-D Metallic Chains on Si(100) by Means of nc-AFM and DFT, M. Setvin, M. Ondracek, P. Mutombo, Z. Majzik, P. Jelinek, Institute of Physics of ASCR, Czech Republic

Scanning Probe techniques are widely used to image atomic and electronic structure of surfaces and nanostructures. However atomic and chemical resolution of complex nanostructures (e.g. molecules, nanoparticles or nanowires) is still the large challenge. Several methods (see e.g. [1-3]) have been already proposed to achieve the single-atom chemical resolution. In the work [3] it was showed that the single-atom chemical identification can be achieved via force-site spectroscopy measurements using Frequency Modulation Atomic Force Microscopy (FM-AFM). The validity of the method was demonstrated on semiconductor surface alloy composed of isovalent species (Si, Sn and Pb). In this particular case, the valence electrons of surface atoms possess very similar electronic structure close to sp³ hybridization with characteristic dangling bond state. Hence the maximum short-range force is mainly driven by the position of the dangling bond state with respect to the Fermi level.

In this work, we investigated atomic and chemical structure of heterogeneous 1-D chains made of III and IV group metals grown on Si(100) surface [4] by means of room-temperature (RT) FM-AFM measurements combined with DFT simulations. Here 1D chains consist of heterogeneous buckled-dimer structures with unknown chemical ordering. What more, the presence of buckled dimmers composed by chemical species of different valence makes this system very challenging for true atomic and chemical resolution by means of SPM.

In this contribution, we will show first that FM-AFM technique even at RT is able to achieve atomic resolution of individual atoms forming dimmerrows, much superior to the contrast obtained by the traditional STM technique. Secondly, we will demonstrate that the single-atom chemical identification is still possible combining the force-site spectroscopy at RT with DFT simulations even in such complex systems as the heterogeneous 1D metallic chains.

[1] M. Schmid, H. Stadler, P. Varga Phys. Rev. Lett., 70, p. 1441 (1993)

[2] L. Gross et al, Science 325, 5944 (2009).

[3] A. Foster et al Phys. Rev. Lett. 102, 256103 (2009).

[4] Y. Sugimoto, P. Pou, M. Abe, P. Jelinek, R. Perez, S. Morita, O. Custance, Nature 446, 64 (2007)

[5] L. Magaud, A. Pasturel, and J.-Y. Veuillen, Phys. Rev. B 65, 245306 (2002).

4:00pm SP+AS+BI+ET+MI+NS-TuA7 Simple Routes to High Speed and Super Resolution AFM, J.K. Hobbs, University of Sheffield, UK INVITED

Over the past two decades atomic force microscopy has developed to become the workhorse of molecular nanotechnology. However, despite this success, it has failed to deliver consistently in two areas where it arguably has most potential, namely sub-molecular resolution imaging and the following of processes in real time. Here our work to tackle these challenges will be discussed.

We have developed a new approach to reaching high resolution within a conventional AFM, based on torsionally driven T-shaped cantilevers, dubbed "torsional tapping AFM". The use of torsional oscillations gives improved dynamics (high Q-factor, high frequency), without excessively increasing the spring constant. The small offset of the tip from the axis of rotation gives improved lever sensitivity. Combined, these result in an approximately 12 fold improvement in sensitivity when compared to the same AFM with a conventional tapping cantilever. This improved sensitivity allows ultra-sharp whisker tips to be used in a routine manner, giving true molecular resolution even on soft materials presenting surfaces with tens of nanometres of topography. For example, individual polyethylene chains both in the crystalline phase, and at the interface with the amorphous phase, can be clearly imaged in a conventionally processed sample of plastic, with polymer chain-to-chain resolution down to 0.37 nm [1]. Data from semi-crystalline polymers to naturally occurring protein crystals will be presented.

High speed AFM requires methods for scanning rapidly, for maintaining tip-sample contact ("feedback"), and for constructing the topography image. We have shown that resonant scanners [2] give a robust method for rapid scanning. In a conventional AFM the feedback and the topographic image are inextricably linked. However, this places a limit on scan speed as it demands that the tip has reached equilibrium at each point on the image if the height is going to be accurately obtained. We have adopted a different approach, in which the height of the tip is directly measured using an interferometric approach, freeing the feedback loop to minimising tip-sample forces. This allows topographic images with height traceable to the wavelength of the interferometric laser to be obtained at imaging rates greater than one frame a second. Coupled with resonant scanners, giving scan areas up to 40×40 um² an AFM platform capable of in-line industrial applications is obtained.

1. Mullin, N.; Hobbs, J. K., Phys Rev Lett 2011,107

2. Humphris, A. D. L.; Miles, M. J.; Hobbs, J. K Appl Phys Lett 2005,86 (3)

4:40pm SP+AS+BI+ET+MI+NS-TuA9 A Scanning Probe Microscopy Study of Trimesic Acid Self-Assembly on Highly Oriented Pyrolytic Graphite, V. Korolkov, S. Allen, C.J. Roberts, S.J.B. Tendler, The University of Nottingham, UK

We have investigated trimesic acid (1,3,5-benzenetricarboxylic acid, TMA) adsorption on highly oriented pyrolytic graphite (HOPG) surfaces from aqueous medium at room temperature. Both atomic force (Peak Force Tapping mode) and scanning tunnelling microscopy were utilized to follow the adsorption dynamics and molecular arrangements. A chicken-wire arrangement for adsorbed molecules with an average pore size of 11 ± 1 Å was established and observed using both scanning techniques. We found that this structure forms a monolayer within ~ 100 seconds of exposure of the HOPG surface to $50\mu M$ TMA solution in H2O. The monolayer structure was found to be stable for at least 48h under ambient conditions. STM was observed to lead to some desorption of TMA from a dynamically formed TMA film, and was only able to image the monolayer of TMA molecules in intimate contact with the HOPG. AFM revealed that TMA films formed using higher concentrations or longer adsorption times formed multilayers with similar molecular spacings and displayed an island growth morphology.

We have achieved an excellent resolution on an ambient running AFM. We have demonstrated that the combination of STM and AFM is essential, if not a must, to look at ultimate monolayers in the ambient conditions. Overall a facile green chemistry method for TMA monolayer fabrication from aqueous media on a HOPG surface has been established.

5:00pm SP+AS+BI+ET+MI+NS-TuA10 Understanding the Role of the Probe in SPM Imaging of Metal Oxides: New Opportunities for In-Depth Surface Analysis, H. Mönig, Univ. of Münster, Germany, M. Todorovic, Univ. Autónoma de Madrid, Spain, M.Z. Baykara, Yale Univ., T.C. Schwendemann, Southern Connecticut State Univ., J. Götzen, Ö. Ünverdi, E.I. Altman, Yale Univ., R. Perez, Univ. Autonoma de Madrid, Spain, U.D. Schwarz, Yale Univ.

Metal oxide surfaces play an indispensible role in a number of catalytic processes of technological and scientific importance. A fundamental understanding of the role that metal oxide surfaces play in such applications requires an experimental technique that allows analyzing chemical and electronic surface properties down to the atomic scale. The powerful method of three-dimensional atomic force microscopy (3D-AFM) in combination with scanning tunneling microscopy (STM) can be used towards this goal with great success. However the interpretation of results is not straightforward, particularly because the structure and chemistry of the probe tip employed in the experiments influences the measured data.

In this talk, using a combination of experimental STM data and density functional theory (DFT) calculations, we will study the effect of changing the tip structure and chemistry, as well as imaging parameters such as tipsample distance and bias voltage on STM images obtained on the model surface of Cu(100)-O, a surface oxide layer consisting of nearly co-planar copper (Cu) and oxygen (O) atoms. We observe that STM image contrasts and atomic species with highest tunneling probability vary greatly with changing tip properties and imaging parameters. Reasonable matches between calculated and experimentally recorded STM images are observed, allowing the determination of particular tip models used in the experiments. Additionally, the effect of rotating the model tip structures with respect to the sample surface results in asymmetric features in simulated STM images, reproducing certain peculiar patterns observed experimentally. To sum up, the results presented here underline the significant role that the tip plays in SPM measurements and describe potential routes to optimize the gathered information through deliberate manipulation of tip properties as well as imaging parameters.

5:20pm SP+AS+BI+ET+MI+NS-TuA11 Characterizing the Best Tips for NC-AFM Imaging on Metal Oxides with Force Spectroscopy and Theoretical Simulations, D. Fernandez-Torre, Universidad Autónoma de Madrid, Spain, A. Yurtsever, Osaka University, Japan, P. Pou, Universidad Autónoma de Madrid, Spain, Y. Sugimoto, M. Abe, S. Morita, Osaka University, Japan, R. Perez, Universidad Autónoma de Madrid, Spain

Metal oxides play a key role in a wide range of technological applications. To optimize their performance, it is essential to understand their surface properties and chemistry in detail. Noncontact atomic force microscopy (nc-AFM) provides a natural tool for atomic-scale imaging of these insulating materials. Some of these materials, including ceria (CeO2), and particularly titania (TiO2), have been extensively studied with nc-AFM in the last few years. Experiments on the rutile TiO2(110) surface show, at variance with STM, that a variety of different contrasts can be obtained, and frequent changes among different imaging modes are observed during scanning. The two most common contrasts are the "protrusion" and the "hole" mode imaging modes, that correspond, to imaging bright the positive or the negative surface ions respectively, but other contrasts like the "neutral" mode and the "all-inclusive" mode –where all the different chemical species and defects are imaged simultaneously—have been also identified.

Understanding the image contrast mechanisms and characterizing the associated tip structures is crucial to extract quantitative information from nc-AFM measurements and to identify the nature of the observed defects. While in many cases the same nc-AFM image can be explained by different models, and even different underlying tip-sample interactions, we show here that the combination of force spectroscopy (FS) measurements and first-principles simulations can provide an unambiguous identification of the tip structure and the image contrast mechanism. In particular, we show that the best tips to explain the protrusion and hole mode forces are TiOxbased clusters differing in just one H atom at the tip apex, discarding previously proposed Ti-terminated tips that would lead to forces much larger than the ones observed in the experiments. The less frequent neutral and all-inclusive images are associated to Si tips where contamination is limited to just an O atom or OH group at the apex. These models provide a natural explanation for the observed contrast reversals by means of H transfer to/from the tip, an event that we indeed observe in our simulations. As tip contamination by surface material is common while imaging oxides, we expect these tips and imaging mechanisms to be valid for other oxides. Our results for the imaging of CeO2 surfaces and of metal atoms (K, Pt) adsorbed on TiO2 support this conclusion.

5:40pm SP+AS+BI+ET+MI+NS-TuA12 Direct Probe of Interplay between Local Structure and Superconductivity in FeTe_{0.55}Se_{0.45}, *M.H. Pan*, *W.Z. Lin*, *Q. Li*, *B.C. Sales*, *S. Jesse*, *A.S. Sefat*, *S.V. Kalinin*, Oak Ridge National Laboratory

A key challenge in high-temperature superconductivity is to determine the role of local crystallographic structure and chemical effects on the critical temperature, T_c superconducting Iron chalcogenide superconductors ('11') are ideal model systems for deciphering the role of local effects on the superconductivity, primarily because they cleave leaving non-polar surfaces unlike other families of iron arsenide superconductors ('1111' or '122') and cuprates . Here, we explore the interplay between local crystallographic structure, composition and local electronic and superconductive properties. Direct structural analysis of scanning tunneling microscopy (STM) data allows local lattice distortions and structural defects across a FeTe_{0.55}Se_{0.45} surface to be explored on a single unit-cell level. Concurrent superconducting gap (SG) mapping reveals suppression of the SG at well-defined structural defects, identified as a local structural distortion (Guinier-Preston zone). The strong structural distortion is related to the vanishing of the superconducting state. This study provides insight into the origins of superconductivity in iron chalcogenides by providing an example of atomic-level studies of the structure-property relationship.

Wednesday Morning, October 31, 2012

Magnetic Interfaces and Nanostructures Room: 6 - Session MI-WeM

Topological Insulators and Rashba

an information carrier.

Moderator: M. Donath, Muenster University, Germany, E. Vescovo, Brookhaven National Laboratory

8:00am MI-WeM1 UP or DOWN? Rashba-type Spin Structures in spand d-derived Surface States Below and Beyond the Fermi Level, M. Donath, S.D. Stolwijk, A. Zumbülte, S.N.P. Wissing, Ch. Langenkämper, A.B. Schmidt, P. Krüger, Muenster University, Germany, K. Miyamoto, K. Shimada, A. Kimura, Hiroshima University, Japan, K. Sakamoto, Chiba University, Japan, R.C. Hatch, P. Hofmann, Aarhus University, Denmark Rashba-type spin splittings in the surface electronic structure of heavy elements and topological insulators are a hot topic of today's research in condensed matter physics. The interest is guided by possible applications of these materials in spintronic devices, in which the electron spin is used as

In this talk, I will present several experimental studies of surface states of different origin and with distinct spin configurations. At W(110), a spinpolarized Dirac-cone-like surface state with *d* character was identified, which appears below the Fermi level in a spin-orbit-induced symmetry gap of the projected bulk-band structure [1]. At Tl/Si(111), an unoccupied surface state with a spin-dependent energy splitting of more the 0.5 eV exhibits a distinct spin structure around the K point, leading to almost complete spin polarization at the Fermi level. Furthermore, the spin-dependent unoccupied electron states of the topological insulator Bi₂Se₃(111) were studied as a function of different preparation conditions. Making combined use of direct and inverse photoemission, we were able to characterize the electronic states below and beyond the Fermi level.

[1] K. Miyamoto et al., Phys. Rev. Lett. 108, 066808 (2012).

8:20am MI-WeM2 Scanning Tunneling Spectroscopy of Topological Insulators' Electrically Tunable Electronic Structure, *N. Levy*, Center for Nanoscale Sci. and Tech. / NIST, *T. Zhang*, Center for Nanoscale Sci. and Tech. / NIST and Maryland NanoCenter / Univ. of Maryland, *J. Ha*, Center for Nanoscale Sci. and Tech. / NIST and Seoul National Univ., Korea, *Y. Kuk*, Seoul National Univ., Republic of Korea, *J.A. Stroscio*, Center for Nanoscale Sci. and Tech. / NIST

Three-dimensional (3D) topological insulators (TI) are a new state of matter with a bulk band gap but topologically protected gapless surface states. These protected surface states are massless helical Dirac fermions which are predicted to host many striking quantum phenomena [1]. Angle resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy (STM) measurements confirmed the existence of these surface states and their helical spin structure [1]. All the 3D TI materials to date have an initial doping level which places the Dirac point away from the Fermi level. Initial studies used chemical doping to align the surface states within the bulk band gap. A preferable method to realize the host of new phenomena in TI materials is to electrically tune the carrier density using the field effect from a gate electrode, as demonstrated in three terminal transport experiments [2]. However, the combination of local probe studies with samples containing low defect concentrations and a tunable carrier density remains a challenge, due to the chemical reactivity of the TI surfaces which precludes ex-situ fabrication and processing of the unprotected films.

In this talk we present new results on atomically flat Bi₂Se₃ and Sb₂Te₃ films grown on SrTiO₃ substrates using Molecular Beam Epitaxy (MBE). SrTiO₃ has a very large dielectric constant of $\sim 10^4$ at 4 K [3], allowing tuning of the TI Dirac point and carrier density even with a relatively thick dielectric of 100 µm. The SrTiO3 substrates were pre-patterned with platinum electrodes and mounted in specially designed sample holders, allowing us to in-situ control the carrier density with a back gate on in-situ grown films, avoiding any ex-situ post processing of the samples. As a result, we are able to continuously change the carrier density and observe the local electronic structure of pristine grown TI films. Initial measurements at 5 K are focused on very thin films of 2 to 10 quintuple layers. Scanning tunneling spectroscopy measurements of the thin film's surface electronic structure allow us to study the gate's efficiency vs. local film thickness in a single sample. We find that the efficiency of gating the top surface state's electronic structure depends on the film thickness, with a decreasing efficiency for thicker films. In addition, we observe substantial differences in gating between Bi₂Se₃ and Sb₂Te₃.We will discuss these results and models of the gating of carriers in the bottom and top surface states through the bulk films at different bulk carrier densities.

[1] Rev. Mod. Phys. 82 3045 (2010)
[2] Nano Lett., 10 (12), 5032 (2010)
[3] Phys. Rev. B 19, 3593–3602 (1979)

11:20am MI-WeM11 Scanning Tunneling Microscopy Observation of the Superconducting Gap in Cu_xBi₂Se₃, *J. Ha*, Center for Nanoscale Sci. and Tech. / NIST and Seoul National Univ., *N. Levy*, Center for Nanoscale Sci. and Tech. / NIST, *T. Zhang*, Center for Nanoscale Sci and Tech. / NIST and Maryland NanoCenter / Univ. of Maryland, *R.L. Kallaher*, *F. Sharifi, A.A. Talin*, Center for Nanoscale Sci. and Tech. / NIST, *Y. Kuk*, Seoul National Univ., Republic of Korea, *J.A. Stroscio*, Center for Nanoscale Sci. and Tech. / NIST

The discovery of topological insulators has triggered the search for new topological states of matter. A topological superconductor is one such state, characterized by the existence of an unconventional superconducting gap in the bulk, and gapless Andreev bound states on the surface. Recently, Cu intercalated Bi₂Se₃ (Cu_xBi₂Se₃) was found to be superconducting with $T_c \approx 3.8~K~[1]$, and is considered a prime candidate for topological superconductivity due to its peculiar band structure and strong spin-orbit coupling. A recent point contact measurement observed zero-bias conductance peaks, claiming these as evidence of surface Andreev bound states, and angle resolved photoemission spectroscopy has revealed the preservation of the topological surface states at the Fermi level [2, 3]. However, direct measurement of the superconducting gap in this material has not been reported.

In this work, we use an ultra-low temperature scanning tunneling microscope [4] to investigate the superconducting properties of a cleaved Cu_xBi₂Se₃ bulk crystal. The crystal was synthesized by electrochemical intercalation of Cu atoms into a previously synthesized Bi₂Se₃ crystal. We observe a superconducting gap in scanning tunneling spectroscopy (STS) measurements. We estimate the size of the gap to be 0.35 meV from a preliminary BCS fit of the superconducting gap. STS measurements under a magnetic field show a complete suppression of the superconducting gap at a critical field of ≈ 1.5 T. Significant inhomogeneity is observed in the material with spatial variations of the superconducting gap. We will discuss these observations in the context of current theories of topological superconductors.

[1] Y. S. Hor et al., Phys. Rev. Lett. 104, 057001 (2010)

[2] L. A. Wray et al., Nat. Phys. 6, 855–859 (2010)

[3] S. Sasaki et al., Phys. Rev. Lett. 107, 217001 (2011)

[4] Y. J. Song et al., Rev. Sci. Instrum. 81, 121101 (2010)

Scanning Probe Microscopy Focus Topic Room: 16 - Session SP+AS+BI+ET+MI+NM+NS+SS+TF-WeM

Probe-Sample Interactions, Nano-Manipulation and Fabrication

Moderator: S. Allen, The University of Nottingham, UK, A.-P. Li, Oak Ridge National Laboratory

8:20am SP+AS+BI+ET+MI+NM+NS+SS+TF-WeM2 Controlled Coupling of Silicon Atomic Quantum Dots at Room Temperature: A Basis for Atomic Electronics?, *R.A. Wolkow*, University of Alberta and The National Institute for Nanotechnology, Canada, *J. Pitters*, The National Institute for Nanotechnology, Canada, *G. DiLabio*, *M. Taucer*, *P. Piva*, *L. Livadaru*, University of Alberta and The National Institute for Nanotechnology, Canada Institute for Nanotechnology, Canada Institute for Nanotechnology, Canada Institute for Nanotechnology, Canada Institute for

Quantum dots are small entities, typically consisting of just a few thousands atoms, that in some ways act like a single atom. The constituent atoms in a dot coalesce their electronic properties to exhibit fairly simple and potentially very useful properties. It turns out that collectives of dots exhibit joint electronic properties of yet more interest. Unfortunately, though extremely small, the finite size of typical quantum dots puts a limit on how close multiple dots can be placed, and that in turn limits how strong the coupling between dots can be. Because inter-dot coupling is weak, properties of interest are only manifest at very low temperatures (milliKelvin). In this work the ultimate small quantum dot is described – we replace an "artificial atom" with a true atom - with great benefit. It is demonstrated that the zero-dimensional character of the silicon atom dangling bond (DB) state allows controlled formation and occupation of a new form of quantum dot assemblies - at room temperature. Coulomb repulsion causes DBs separated by less than ~2 nm to experience reduced localized charge. The unoccupied states so created allow a previously unobserved electron tunnel-coupling of DBs, evidenced by a pronounced change in the time-averaged view recorded by scanning tunneling microscopy. It is shown that fabrication geometry determines net electron occupation and tunnel-coupling strength within multi-DB ensembles and moreover that electrostatic separation of degenerate states allows controlled electron occupation within an ensemble.

Some speculation on the viability of a new "atomic electronics" based upon these results will be offered.

9:00am SP+AS+BI+ET+MI+NM+NS+SS+TF-WeM4 Atomic Forces and Energy Dissipation of a Bi-Stable Molecular Junction, C. Lotze, Freie Universtiät Berlin, Germany, M. Corso, K.J. Franke, F.V. Oppen, J.I. Pascual, Freie Universität Berlin, Germany

Tuning Fork based dynamic STM/AFM is a well established method combining the advantages of scanning tunneling and dynamic force microscopy. Using tuning forks with high stiffness, stable measurements with small amplitudes, below 1 Å can be performed. In this way, conductance and frequency shift measurements of molecular junction can be obtained simultaneously [1] with intramolecular resolution [2].

One of the most intriguing aspects of molecular junctions relates to the effect of structural bi-stabilities to the properties of the junction. These lead, for example, to conductance fluctuations, telegraph noise and the possibility to switch the electrical transport through the junction.

In this presentation, we characterize a model bi-stable molecular system using dynamic force spectroscopy. The effect of current-induced stochastic fluctuations of conductance are correlated with fluctuations in force. In our experiment we identified the last from both, frequency shifts and energy dissipation measurements, picturing a regime in which electrical transport and mechanical motion are coupled.

[1] N. Fournier et. al, PhysRevB 84, 035435 (2011),

[2] L. Gross et. al, Science 324, 1428 (2009)

9:20am SP+AS+BI+ET+MI+NM+NS+SS+TF-WeM5 Acetylene on Cu(111): Imaging a Molecular Pattern with a Constantly Rearranging Tip, Y. Zhu, J. Wyrick, K.D. Cohen, K. Magnone, C. Holzke, D. Salib, Q. Ma, D.Z. Sun, L. Bartels, University of California Riverside

Abstract: Using variable temperature STM and DFT simulation, we identify the phases of acetylene adsorbed on the Cu(111) surface. Depending on the coverage, a diffraction-derived surface pattern of acetylene on Cu(111) is validated by STM. The modification of the STM image transfer function through the adsorption of an acetylene molecule onto the tip apex is taken into account. In this case, the images of acetylene patterns on Cu(111) also include direct evidence of **the rotational orientation and dynamics of the acetylene species attached to the tip apex**. DFT modeling of acetylene/Cu(111) reveals that the molecular orientation and separation is governed by a balance of repulsive interactions associated with stress induced in the top surface layer and attractive interactions mediated by the electronic structure of the substrate. Computationally modeling of the substrate with 3 layers obtains the periodicity of the intermolecular interaction that provides a theoretical underpinning for the experimentally observed molecular arrangement.

9:40am SP+AS+BI+ET+MI+NM+NS+SS+TF-WeM6 Atomic Scale Imaging and Electronic Structure of Trimethylaluminum Deposition on III-V Semiconductor (110) Surfaces, *T.J. Kent**, *M. Edmonds, E. Chagarov, A.C. Kummel*, University of California San Diego

Silicon based metal oxide semiconductor field effect transistors (Si-MOSFETs) are quickly approaching their theoretical performance limits, as a result many semiconductors are being explored as an alternative channel material for use in MOSFETs. III-V semiconductors are an appealing alternative to Si because of their higher electron mobilities. The limiting factor in III-V based MOSFET performance is defect states which prevent effective modulation of the Fermi level. The InGaAs (001) As-rich (2x4) surface contains two types of unit cells: ideal unit cells with double As-dimers and defect unit cells with single As-Dimers. The missing As-dimer unit cells, which comprise ~50% of the surface, are believed to cause electronic defect states at the semiconductor. *In-situ* scanning tunneling microscopy and spectroscopy (STM/STS) and density function theory

(DFT) modeling show that TMA readily passivates the As-As dimers in the ideal unit cell but the missing InGaAs(001)-2x4 may not be fully passivated by TMA. To improve the electronic structure of the interface, the sidewalls of the finFETs on InGaAs(001) can be fabricated along the (110) direction. The (110) surface contains only buckled III-V heterodimers in which the lower group III atom is sp2 hybridized with an empty dangling bond and the upper group V atom is sp3 hybridized with a full dangling bond. This results in an electrically unpinned surface.

To investigate the benefits of using a (110) surface as a channel material, the atomic and electronic structure of the ALD precursor trimethylaluminum (TMA) monolayer deposited on III-V (110) surfaces has been studied using *in-situ* STM and STS. Both GaAs and InGaAs samples were studied. GaAs wafers were obtained from Wafertech with a Si doping concentration of 4x1018/cm3. The (001) samples were cleaved *in-situ* to expose the (110) surface. Samples were transferred to the STM chamber (base pressure 1x10-11 torr) where the atomic bonding structure of the precursor monolayer unit cell was determined. STS, which probes the local density of states (LDOS), was used to determine Fermi level pinning. A model of TMA chemisorption was developed in which TMA chemisorbs between adjacent As atoms on the surface, giving a highly ordered monolayer with a high nucleation density which could allow for aggressive effective oxide thickness (EOT) scaling.

SP+AS+BI+ET+MI+NM+NS+SS+TF-WeM9 10:40am A New Experimental Method to Determine the Torsional Spring Constants of Microcantilevers, G. Haehner, J.D. Parkin, University of St Andrews, UK Cantilever based technologies have seen an ever increasing level of interest since the atomic force microscope (AFM) was introduced more than two decades ago. Recent developments employ microcantilevers as stand-alone sensors by exploiting the dependence of their oscillating properties on external parameters such as adsorbed mass [1], or the density and the viscosity of a liquid environment [2,3]. They are also a key part in many microelectromechanical systems (MEMS) [4]. In order to quantify measurements performed with microcantilevers their stiffness or spring constants have to be known. Following calibration of the spring constants a change in oscillation behavior can be quantitatively related to physical parameters that are probed. The torsional modes of oscillation have attracted significant attention due to their high sensitivity towards lateral and friction forces, and recent developments in torsional-tapping AFM technology [5]. However, the methods available to determine the torsional spring constants experimentally are in general not simple, not very reliable, or risk damage to the cantilever [6].

We demonstrate a new method to determine the spring constants of the torsional modes of microcantilevers experimentally with high accuracy and precision. The method is fast, non-destructive and non-invasive. It is based on measuring the change in the resonance frequencies of the torsional modes as a function of the fluid flow escaping from a microchannel. Results for rectangular cantilevers will be presented and compared to results obtained with other methods [7].

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11:00am SP+AS+BI+ET+MI+NM+NS+SS+TF-WeM10 A Torsional Device for Easy, Accurate and Traceable Force Calibration of AFM Cantilevers, J.F. Portoles, P.J. Cumpson, Newcastle University, UK

Accurate measurement of biologically-relevant forces in the range of pN to μN is an important problem in nanoscience.

A number of force probe techniques have been applied in recent years. The most popular is the Atomic Force Microscope (AFM). Accuracy of force measurement relies on calibration of the probe stiffness which has led to the development of many calibration methods[1], particularly for AFM microcantilevers. However these methods typically exhibit uncertainties of at best 15% to 20% and are often very time consuming. Dependency on material properties and cantilever geometry further complicate their application and take extra operator time. In contrast, one rapid and straightforward method involves the use of reference cantilevers (the "cantilever-on-cantilever" method) or MEMS reference devices. This

^{*} ASSD Student Award Finalist

approach requires that a calibrated reference device is available, but it has been shown to be effective in providing measurement traceability[2].

The main remaining difficulty of this approach for typical users is the positional uncertainty of the tip on the reference device, which can introduce calibration uncertainties of up to around 6%. Here we present a new reference device based on a torsional spring of relatively large dimensions compared to the typical AFM cantilever and demonstrate how it is calibrated. This method has the potential to calibrate the reference device traceably[3] to the SI with a 1% accuracy by applying techniques typically used for the characterisation of micromechanical devices. The large dimensions of the device reduce the positional uncertainty below 1% and simultaneously allow the use of the device as an effective reference array with different reference stiffnesses at different positions ranging from 0.090 N/m to 4.5 N/m

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11:20am SP+AS+BI+ET+MI+NM+NS+SS+TF-WeM11 Nanoscale Surface Assembly by Single-Molecule Cut-and-Paste, H.E. Gaub, Ludwig-Maximilians Universitat, Germany INVITED Bottom up assembly of functional molecular ensembles with novel properties emerging from composition and arrangement of its constituents is a prime goal of nanotechnology. With the development of Single-Molecule Cut-and-Paste (SMC&P) we provided a platform technology for the assembly of biomolecules at surfaces. It combines the A-positioning precision of the AFM with the selectivity of DNA hybridization to pick individual molecules from a depot chip and allows to arrange them on a construction site one by one. An overview on different applications of this technology will be given in this talk. One recent example demonstrates the functional of receptors for small molecules. By SMC&P we assembled binding sites for malachite green in a molecule-by-molecule assembly process from the two halves of a split aptamer. We show that only a perfectly joined binding site immobilizes the fluorophore and enhances the fluorescence quantum yield by several orders of magnitude. To corroborate the robustness of this approach we produced a micron-sized structure consisting of more than 500 reconstituted binding sites. To the best of our knowledge this is the first demonstration of a one by one bottom up functional bio-molecular assembly. Figure included in supplemental document. S. Kufer, Puchner E. M., Gumpp H., Liedel T. & H. E. Gaub Science (2008), Vol 319, p 594-S. Kufer, Strackharn, M., Stahl S.W., Gumpp H., Puchner E. M. & H. E. Gaub Nature Nanotechnology (2009), Vol 4, p 45-M. Erdmann, R. David. A.N. Fornof, and H. E. Gaub, Nature Chemistry (2010), Vol 2, p 755-M. Strackharn, S. Stahl, E. Puchner & H.E. Gaub, Nanoletters (2012) in press

Wednesday Afternoon, October 31, 2012

Magnetic Interfaces and Nanostructures Room: 6 - Session MI+OX-WeA

Spintronics, Magnetoelectrics, Multiferroics

Moderator: G.J. Mankey, University of Alabama

2:00pm MI+OX-WeA1 Imaging of Temperature-Driven Nucleation of Ferromagnetic Domains in FeRh Thin Films, C. Baldasseroni, C. Bordel, Univ. of California Berkeley, A.X. Gray, SLAC National Accelerator Lab, A.M. Kaiser, Peter-Grünberg-Institut, Germany, F. Kronast, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany, J. Herrero-Albillos, Centro Univ. de la Defensa, Spain, C.M. Schneider, Peter-Grünberg-Institut, Germany, C.S. Fadley, Lawrence Berkeley National Lab, F. Hellman, Univ. of California Berkeley

Equiatomic FeRh is a unique material that undergoes a first order antiferromagnetic (AF) to ferromagnetic (FM) transition just above room temperature (near 350 K). This phase transition can be driven by temperature or magnetic field and is coupled to a lattice expansion. Current investigations of this unique transition range from the fundamental understanding of the origin and nature of the transition to applications associated with the transition such as a giant magnetocaloric effect.

FeRh has been studied in the bulk for over 50 years and most recently in thin film form, where the transition temperature has been shown to be sensitive to changes in composition and substrate-induced strain as well as structural and chemical order. FeRh thin films are also a promising candidate for heat-assisted magnetic recording in an exchange-spring system with a hard magnetic layer (for example FePt). Understanding the magnetic domain structure of FeRh and the mechanisms of the transition at the microscopic level involving nucleation and growth of magnetic domains as a function of temperature is vital for its further application to magnetic storage technology. Although many experimental studies of the transition have been recently performed on FeRh thin films, most of them focus on macroscopic measurements. Only a few studies have attempted at imaging domains through the transition but these have been limited to magnetic force microscopy (MFM) on bulk samples and were limited by lack of temperature control which prevented a study of the nucleation and growth across the full transition.

We used x-ray magnetic circular dichroism and photoemission electron microscopy to study the evolution of ferromagnetic domains across the temperature-driven AF to FM phase transition in uncapped and capped epitaxial FeRh thin films. The coexistence of the AF and FM phases was evidenced across the broad transition and the different stages of nucleation, growth and coalescence were observed. We also found that the FM phase nucleates into single domain islands and the width of the transition of the individual nuclei is sharper than that of the macroscopic transition.

2:20pm MI+OX-WeA2 Magnetic Properties of Cobalt and Permalloy Thin Films Grown on Self-Assembled Monolayers by Physical Vapor Deposition, G.J. Szulczewski, S. Schafer, B. Khodadadi, T. Mewes, J. Kreil, E. Ellingsworth, K. Anderson, The University of Alabama

In this talk we will present results from a study to understand how terminal functional groups in self-assembled monolayers (SAMs) influence the growth and subsequent magnetic properties of Co and NiFe (permalloy) thin films. Self-assembled monolayers were made from both aryl and alkyl carboxylic acids adsorbed onto oxidized aluminum surfaces. The SAMs were characterized by contact angle measurements and x-ray photoelectron spectroscopy. The magnetic properties of the thin films were characterized by ferromagnetic resonance spectroscopy. In general we find that reactive functional groups, for example thiols, cause the metals to grow as continuous films. In contrast, deposition of the metals onto non-reactive functional groups, for example methyl, leads to penetration of metal atoms through the SAM and cluster formation. The permalloy films are superparamagnetic below ~ 4 nm, while Co films are ferromagnetic at room temperature. The coercivity of the films is also found to vary with functional group. In the case of halide substituents, for example, flouro, chloro, bromo, and iodo on the aryl carboxylic SAMs, there is also a correlation between the magnetic properties of cobalt thin films and the strength of the carbon-halogen bond energy. Cobalt deposited onto SAMs with terminal C-F bonds tends to be non-reactive, while reactive toward C-I bonds. Not only do these reactivity patterns influence the magnetic properties of the thin film, but also they result in a measurable change in the resistance of tunnel junctions bearing these SAMs.

2:40pm MI+OX-WeA3 Synthesis and Fundamental Properties of Fe16N2 Films - New Excitements of Fe16N2 Research and a 40-year Mystery, J.-P. Wang, University of Minnesota INVITED

Pursuing magnetic materials with giant saturation magnetization (Ms) has huge impacts both scientifically and technologically. However, this effort has been fundamentally shadowed for decades by the classical itinerant magnetism theory. So far, the highest 4piMs value that can be predicted by first principles calculation is 2.45 T for Fe65Co35 alloy.

In 1972, Kim and Takahashi firstly reported a material with a giant saturation magnetization (4piMs ~ 2.9 T), Fe16N2, that surpasses Fe65Co35 alloy. Thereafter, various groups in the world have investigated the formation of Fe16N2 samples including films and particles by a variety of means. Unfortunately, experimentally reported 4piMs values are largely inconsistent ranging from 2.2 T up to 2.9 T. Investigators, including theoreticians, weighted in on one side of this question or the other. In particular, at the annual conference on Magnetism and Magnetic Materials in 1996, a symposium was held on the topic Fe16N2. Key research teams on this topic presented apparently conflicting views on the synthesis and understanding of this material. No decisive conclusion was drawn on whether Fe16N2 has giant saturation magnetization at the moment. Since then, this research topic has been dropped by most of magnetic researchers since year 2000.

In 2010, Wang's group has reported the theory and fundamental experimental evidence of the origin of giant saturation magnetization and produced the Fe16N2 thin films with both giant Ms and high anisotropy. In this talk, Dr. Wang will review the history and analyze the previous inconsistencies and obstacles of the Fe16N2 topic in the past 40 years. Then he will present recent progress from his group and his collaborators on this topic. From X-ray magnetic circular Dichorism (XMCD) experiment, polarization-dependent x-ray absorption near edge spectroscopy (EXANE), polarized neutron reflectivity (PNR) and first-principle calculation, it has been both experimentally and theoretically justified that the origin of giant saturation magnetization and large magnetocrystalline anisotropy is correlated with the formation of highly localized 3d electron states in this Fe-N system. Thirdly, high magnetic anisotropy and high spin polarization ratio of Fe16N2 will be reported and discussed, which may lead to many new applications, such as in spintronic device and rare-earth free magnet. Finally remaining fundamental questions and possible approaches to address them will be reviewed and discussed.

This talk is a joint effort with five research teams at ORNL, Argonne National Lab, Brookheaven National Lab and one lab from Netherland.

4:00pm MI+OX-WeA7 Spin Transfer Torque MRAM - Modeling, Experiments and Future Prospects, D. Apalkov, A. Khvalkovskiy, V. Nikitin, S. Watts, A. Driskill-Smith, D. Lottis, R. Chepulskyy, V. Voznyuk, X. Tang, K. Moon, E. Chen, C.M. Park, M. Krounbi, Grandis, Inc. INVITED Spin transfer torque magnetic random access memory (STT-MRAM) is a new and promising memory technology that features fast read and write times, small cell sizes of < 6F2, nonvolatility, radiation hardness and low power consumption.

In this work, we will go over the fundamental physics of magnetoresistance and spin transfer torque effects - key scientific phenomena required for STT-MRAM memory operation. The precursor technology - conventional MRAM - is now successfully used in commercial applications; however it cannot be scaled down to compete with DRAM or Flash technologies. We will go over the Write-Store-Read (WSR) trilemma, which is the challenge to achieve fast and reliable writing, reading and storing information at the same time in STT-MRAM. For a successful product, the desired probability of a switching error at the current deliverable by the transistor should be less than 10-3 for storage-class memory and 10-9-10-18 for working-class memory. Depending on the switching time, two regimes of switching, thermal and precessional, can be identified, and the switching error can dramatically depend not only on the switching regime but also on the switching time within the regime. For the reading process, one critical parameter is read disturb - probability of inadvertent switching of the element during reading operation. For memory applications, this probability has to be smaller than ~10-20 (with some dependence on particular design and array size). For storing the recorded information, the thermal stability parameter, defined as the ratio of energy barrier to kBT is important and typically has to be larger than 60-80 depending on specific application.

STT-MRAM can be implemented in two major realizations: in-plane and perpendicular. For each of them, single and dual MgO designs can be

implemented, with the dual MgO design having up to 50% reduction of the switching current and providing much better switching symmetry than a single one. Special attention will be paid to our recent developments to of in-plane Dual MTJ design. By building special structure with modified reference layers, we were able to extract contributions from each barrier. Even though STT switching current is reduced in Dual design, the quality of the two barriers in currently built structures is deteriorated as compared to single MTJ. Respectively further improvement from Dual designs is expected if the quality of the two barriers is improved.

4:40pm MI+OX-WeA9 Epitaxial Growth of Multiferroic Heterostructures of Magnetic and Ferroelectric Oxides using the Duallaser Ablation Technique, D. Mukherjee, M. Hordagoda, R.H. Hyde, N. Bingham, H. Srikanth, P. Mukherjee, S. Witanachchi, University of South Florida

 $Epitaxial \quad multiferroic \quad PbZr_{0.52}Ti_{0.48}O_3 \quad (PZT)/ \quad CoFe_2O_4 \quad (CFO)/$ La_{0.7}Sr_{0.3}MnO₃ (LSMO) composite thin films were fabricated on singlecrystal SrTiO₃ substrates using the dual-laser ablation process. In this process, the target was initially heated by a pulsed CO₂ laser to produce a transient molten layer, from which a spatially-overlapped and slightly timedelayed pulsed KrF laser initiated the ablation. This not only resulted in a drastic reduction of particulates in the deposited films but also overcame the problem of non-congruent ablation of PZT, due to the high volatility of Pb, leading to stoichiometric PZT film deposition [1]. Moreover, the optimum coupling of the laser energies led to higher ionization of the ablated species particularly atomic oxygen (O) as seen in the optical emission spectra of the plumes. The higher excitation of O led to enhanced gas phase reaction and consequently reduced the oxygen vacancy-related point defects inherent in oxide films. X-ray diffraction (XRD) studies revealed the single crystalline nature and the cube-on-cube epitaxial relationship in the PZT/CFO/LSMO films. Atomic force microscopy revealed surface roughness values as low as 1.6 nm for the top PZT layers. Cross-sectional high resolution transmission electron microscope (HRTEM) images not only evidenced the epitaxial growth but also atomically sharp and flat interfaces with no structural defects (Suppl. PDF). The lattice parameters calculated from the HRTEM images matched well with the values obtained from XRD. Selected area electron diffraction (SAED) patterns showed linear square arrays confirming the single crystalline nature of the interfaces. Magnetization measurements exhibited perpendicular magnetic anisotropy with the easy axis along the film plane for the PZT/CFO/LSMO films, similar to PZT/LSMO bilayer thin films. PZT/CFO/LSMO films showed enhanced inplane saturation magnetization (Ms) values of 360 emu/cm³ as compared to 280 emu/cm3 for PZT/LSMO and larger coercive field of 2.5 kOe as compared to 0.1 kOe for PZT/LSMO thin films. For ferroelectric measurements, top LSMO dot electrodes with 100 µm diameter were deposited using laser ablation to make LSMO/PZT/CFO/LSMO capacitors. Polarization measurements showed well saturated and square hysteresis loops at low nominal switching voltages of 5 V and with higher remnant polarization (P_r) values of 120 μ C/cm² as compared to 90 μ C/cm² for PZT/LSMO thin films.

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MI+OX-WeA10 The Highly Polarized Surface of 5:00pm Magnetoelectric Antiferromagnet, N. Wu, X. He, J. Santana, J. Wang, University of Nebraska-Lincoln, E. Vescovo, Brookhaven National Laboratory, C. Binek, P.A. Dowben, University of Nebraska-Lincoln Manipulation of magnetically ordered states by electrical means is among the most promising approaches towards novel spintronic devices. Electric control of the exchange bias can be realized when the passive antiferromagnetic pinning layer is replaced by a magneto-electric antiferromagnet, like the prototypical magneto-electric Cr2O3(0001). Chromia works well in this case so long as there is also a finite remanent spin polarization at the surface or boundary, which can be achieved by cooling the thin film in the presence of both magnetic and electrics fields. We have demonstrated that a very unusual high polarization can exist at the surface of the Cr₂O₃ (0001) from spin-polarized photoemission [1] and is robust against surface roughness. Both magnetic single domain and multidomains were imaged by magnetic force microscopy and X-ray magnetic circular dichroism - photoemission electron microscopy (XMCD-PEEM) [2] as achieved by field cooling in the presence of electrics fields. The similar boundary magnetization has also been observed on the (110) surface of Fe₂TeO₆ by the XMCD-PEEM, which suggests this possible interface spin polarization to be a more universal phenomenon for magnetoelectric antiferromagnets.

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5:20pm MI+OX-WeA11 Sub-monolayer Spin Rotation of Photoelectrons from FePc on Fe(110), J.E. Rowe, D.B. Dougherty, A.A. Sandin, North Carolina State University, E. Vescovo, Brookhaven National Laboratory

Spin-resolved photoemission at the National Synchrotron Light Source, Brookhaven National Laboratory has been used to study the occupied electronic states of sub-monolayers to multi-layers of iron phthalocyanine (FePc) adsorbed on ~10-20 monolayer epitaxial films on Fe(110) on W(110). We find that the spin-resolved photoemission changes rapidly as a function of coverage and the initial (majority spin axis along [110] rotates by ~ 30 degrees for sub-monolayer coverage and then becomes unpolarized at ~1 monolayer (ML). The coverage is determined by work function measurements which show that the initial work function of clean Fe(110) of 5.0 eV decreases monotonically to a value of ~3.8 eV at a coverage that we assign as ~1 monolayer of FePc. These values were determined from the measurements of the photoelectron spectrum using the low-energy vacuum-level cutoff of a biased sample. We used low intensity light at 41.4 eV photon energy to provide accurate intensity data and a well-defined vacuum-level threshold.

Our spin-resolved data for clean Fe(110) show highly spin-polarized photoelectrons from the Fermi energy to values about 3.5 eV below the Fermi energy for an applied B-field along [110] both for majority-spin and minority-spin electrons. The polarization is about 60% at -3.2 eV below E-Fermi. For 0.13 ML adsorbed FePc the spin polarization is somewhat reduced and is rotated from [110] towards [100] in the plane of the sample. We interpret this rotation as due to a strong coupling of the orbital moment of FePc with the conduction electrons of the Fe substrate. At a coverage of \sim 0.25 ML the polarization is reduced to \sim 0 and then at higher coverage (\sim 1 ML) it increases to about 1/2 of the initial polarization. These data suggest that paramagnetic molecular species are useful for modifying the interfaces of spin-valve devices. A mechanism for this effect will be presented.

MI+OX-WeA12 Magnetic Configurations of Ni₈₀Fe₂₀/Ir 5:40pm Superlattices, G.J. Mankey, University of Alabama, J. Hwang, Lane College, N. Pachauri, E.A. Manoharan, P.R. LeClair, University of Alabama, H. Ambaye, V. Lauter, Oak Ridge National Laboratory Antiferromagnetically coupled superlattices consisting of ferromagnetic (FM) layers separated by nonmagnetic (NM) spacer layers exhibit a wide range of magnetization behavior as a function of applied field. The magnetic configurations depend on the magnetization, thickness and anisotropy of the FM layers and the strength and type of magnetic coupling through the NM layers. The dependence of the magnetic configurations on applied magnetic field can be estimated with one-dimensional micromagnetic models that find the minimum energy configurations of the average magnetization vectors within the ferromagnetic layers1. A set of Ni80Fe20/Ir superlattice samples was designed to compare the measured magnetization curves as a function of applied field to magnetization curves generated by a micromagnetic model. The Ni80Fe20 layers were sputter deposited with an in-plane magnetic field, to induce uniaxial anisotropy within these layers. Both the FM layer thickness and number of superlattice periods were varied. FM layer thicknesses were verified by magnetometry and x-ray reflectivity analysis. The Ir NM layer thickness was tuned to the thickness for maximum antiferromagnetic coupling strength. Ir was chosen because the coupling strength has strong temperature dependence, increasing by about a factor of two as the temperature is reduced from 300 K to 5 K. A detailed comparison of the modeled and experimental magnetization curves enables a parameterization of the micromagnetic model that shows applying a magnetic field generates a complex magnetic structure in finite superlattices for multiple repeats. This complex structure, with twisted magnetic configuration is measured for a 16-repeat superlattice structure using polarized neutron reflectivity. Analysis of the polarized neutron reflectivity data for the applied magnetic field along the hard axis of the FM layers allows the determination of the detailed magnetic configuration.

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The authors gratefully acknowledge financial support from DOE award DE-FG02-08ER46499. Research at Oak Ridge National Laboratory's Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

References:

Scanning Probe Microscopy Focus Topic Room: 16 - Session SP+AS+BI+ET+MI+TF-WeA

Emerging Instrument Formats

Moderator: A. Belu, Medtronic, Inc.

2:00pm SP+AS+BI+ET+MI+TF-WeA1 Electrochemical Strain Microscopy: Nanoscale Imaging of Solid State Ionics, S. Jesse, Oak Ridge National Laboratory INVITED

Electrochemical reactions in solids underpin multiple applications ranging from electroresistive non-volatile memory and neuromorphic logic devices memories, to chemical sensors and electrochemical gas pumps, to energy storage and conversion systems including metal-air batteries and fuel cells. Understanding the functionality in these systems requires probing reversible (oxygen reduction/evolution reaction) and irreversible (cathode degradation and activation, formation of conductive filaments) electrochemical processes. Traditionally, these effects are studied only on the macroscopically averaged level. In this talk, I summarize recent advances in probing and controlling these transformations locally on nanometer level using scanning probe microscopy. The localized tip concentrates an electric field in a nanometer scale volume of material, inducing local ion transport. Measured simultaneously, the electromechanical response (piezo response) or current (conductive AFM) provides the information on bias-induced changes in a material. Here, I illustrate how these methods can be extended to study local electrochemical transformations, including vacancy dynamics in oxides such as titanates, LaxSr1-xCoO3, BiFeO3, and YxZr1-xO2. The formation of electromechanical hysteresis loops indistinguishable from those in ferroelectric materials illustrate the role ionic dynamics can play in piezoresponse force microscopy and similar measurements. In materials such as lanthanum-strontium cobaltite, mapping both reversible vacancy motion and vacancy ordering and static deformation is possible, and can be corroborated by post mortem STEM/EELS studies. The possible strategies for elucidation ionic motion at the electroactive interfaces in oxides using high-resolution electron microscopy and combined ex-situ and in-situ STEM-SPM studies are discussed. Finally, the future possibilities for probing electrochemical phenomena on in-situ grown surfaces with atomic resolution are discussed. This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

2:40pm SP+AS+BI+ET+MI+TF-WeA3 Probing Electrochemical Phenomena in Reactive Environments at High Temperature: *In Situ* Characterization of Interfaces in Fuel Cells, *S.S. Nonnenmann, R. Kungas, J.M. Vohs, D.A. Bonnell*, University of Pennsylvania

Many strategies for advances in energy related processes involve high temperatures and reactive environments. Fuel cell operation, chemical catalysis, and certain approaches to energy harvesting are examples. Scanning probe microscopy provides a large toolbox of local and often atomic resolution measurements of phenomena at a scale that enables understanding of complex processes involved in many systems. Inherent challenges exist, however, in applying these techniques to the realistic conditions under which these processes operate. To overcome some of these challenges, we have designed a system that allows SPM at temperatures to 850° C in reactive gas environments. This is demonstrated with the characterization of an operating fuel cell. Solid oxide fuel cells (SOFCs) offer the highest conversion efficiencies with operating temperatures ranging from 400° C - 1000° C; and operate under variable gaseous fuel environments - H2-based environments (anode side) and O2-based environments (cathode side). Topography and the temperature dependence of surface potential are compared to impedance. While not (yet) at atomic levels of spatial resolution, these probes are at the scale to examine local interface properties.

3:00pm SP+AS+BI+ET+MI+TF-WeA4 High-Resolution Scanning Local Capacitance Measurements, *M. Brukman*, University of Pennsylvania, *S. Nanayakkara*, National Renewable Energy Laboratory, *D.A. Bonnell*, University of Pennsylvania

Spatial variation of dielectric properties often dictates the behavior of devices ranging from field effect transistors to memory devices to organic electronics, yet dielectric properties are rarely characterized locally. We present methods of analyzing 2nd harmonic-based local capacitance measurements achieved through non-contact atomic force microscopy. Unlike contact-based methods, this technique preserves tip shape and

allows the same probe to realize high-resolution topographic imaging and scanning surface potential imaging. We present an improved analysis of the electrical fields between tip and sample, yielding high sensitivity to the capacitance-induced frequency shift.

The techniques are applied to thin-film ceramics (SrTiO2 and HfO2), metals (Pt and Ti), and mixed-phase self-

assembled monolayers to illustrate application over all orders of dielectric constant. Conversion from frequency shift signal to dielectric constant κ is demonstrated, with sub-5 nm spatial resolution and dielectric constant resolution between 0.25 and 1.

4:00pm SP+AS+BI+ET+MI+TF-WeA7 Experimental Calibration of the Higher Flexural Modes of Microcantilever Sensors, J.D. Parkin, G. Hähner, University of St Andrews, UK

Microcantilevers are widely employed as probes not only in atomic force microscopy [1], but also as sensors for mass [2], surface stress [3], chemical identification [3], or in measuring viscoelastic properties of cells [4].

Use of the higher flexural modes of microcantilever sensors is an area of current interest due to their higher Q-factors and greater sensitivity to some of the properties probed [2]. A pre-requirement for their exploitation, however, is knowledge of their spring constants [5]. None of the existing cantilever calibration techniques can calibrate the higher flexural modes easily.

We present a method that allows for the determination of the spring constants of all flexural modes. A flow of gas from a microchannel interacts with the microcantilever causing a measurable shift in the resonance frequencies of all flexural modes [6]. The method is non-invasive and does not risk damage to the microcantilever. From the magnitude of the frequency shifts the spring constants can be determined with high accuracy and precision. Experimental data for the response of the first four flexural modes of microcantilever beams used in AFM with spring constants in the range of ~0.03-90 N/m will be presented.

The spring constants of the first mode determined using our method are compared to those obtained with the Sader method [7]. Finite element analysis computational fluid dynamics (CFD) simulations of the experimental setup are used to provide an insight into the interaction of the flow with the microcantilever.

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4:20pm SP+AS+BI+ET+MI+TF-WeA8 Atomic Imaging with Peak Force Tapping. B. Pittenger, Y. Hu, C. Su, S.C. Minne, Bruker AFM, I. Armstrong, Bruker Nano Surfaces Division

As its name implies, Atomic Force Microscopy (AFM) has long been used to acquire images at the atomic scale. However these images usually only show the lattice of atoms in the crystal and do not show individual atomic defects. In order to achieve atomic resolution, researchers have typically had to design their systems for the ultimate in noise performance, sacrificing ease of use, flexibility, and scan size. Recently we have demonstrated that, by using Peak Force Tapping, our large sample platforms (Dimension Icon, Dimension FastScan) are capable of obtaining atomic resolution imaging along with maps of the tip-sample interaction. Unlike standard TappingMode, or FM-AFM, Peak Force Tapping uses instantaneous force control, allowing the system to be insensitive to long range forces while maintaining piconewton level control of the force at the point in the tapping cycle that provides the highest resolution - the peak force. Since the modulation frequency is far from resonance, the technique is less sensitive to the cantilever thermal noise (Brownian motion). In addition to topography, this technique can provide maps of the interaction between the tip and the sample. This is possible since Peak Force Tapping has access to the instantaneous force between tip and sample at any point in the modulation cycle. To study the details of a tip-sample interaction, Atomic Peak Force Capture can acquire the entire force distance curve used to create the interaction maps. These curves can be exported for easy analysis with models of tip-sample interaction. In this talk we will discuss the latest atomic resolution results using Peak Force Tapping and the implications of this with regard to studies of dissolution, crystallization, ordered liquids, and corrosion.

4:40pm SP+AS+BI+ET+MI+TF-WeA9 Nanoscale Chemical Composition Mapping with AFM-based Infrared Spectroscopy, C.B. Prater, M. Lo, Q. Hu, Anasys Instruments, C. Marcott, Light Light Solutions, B. Chase, University of Delaware, R. Shetty, K. Kjoller, E. Dillon, Anasys Instruments INVITED

The ability to identify material under an AFM tip has been identified as one of the "Holy Grails" of probe microscopy. While AFM can measure mechanical, electrical, magnetic and thermal properties of materials, until recently it has lacked the robust ability to chemically characterize unknown materials. Infrared spectroscopy can characterize and identify materials via vibrational resonances of chemical bonds and is a very widely used analytical technique. We have successfully integrated AFM with IR spectroscopy (AFM-IR) to obtain high quality infrared absorption spectra at arbitrary points in an AFM image, thus providing nanoscale chemical characterization on the sub-100 nm length scale. Employing the AFM-IR technique, we have mapped nanoscale chemical, structural and mechanical variations in multilayer thin films, nanocomposites, polymer blends, organic photovoltaics, and biological materials including hair, skin, and bacterial and mammalian cells. Light from a pulsed infrared laser is directed at a sample, causing rapid thermal expansion of the sample surface at absorbing wavelengths. The rapid thermal expansion creates an impulse force at the tip, resulting in resonant oscillations of the AFM cantilever. The amplitude of the cantilever oscillation is directly related to the infrared absorption properties of the samples, enabling measurements of IR absorption spectra far below the conventional diffraction limit. AFM-IR can be used both to obtain point spectra at arbitrary points and to spatially map IR absorption at selected wavelengths. Simultaneous measurement of the cantilever's contact resonance frequency as excited by the IR absorption provides a complimentary measurement of relative mechanical properties. We have used these techniques to chemically identify individual chemical components in polymer nanocomposites and multilayer films and performed subcellular spectroscopy and chemical imaging on biological cells. Using self-heating probes we have been able to locally modify the state of a semicrystalline polymer and observe the resulting change in absorption spectra on the nanoscale. Using polarization sensitive AFM-IR, we have mapped spatial variations in molecular orientation in electrospun fibers.

5:20pm SP+AS+BI+ET+MI+TF-WeA11 Quantifying Nanomechanical Properties with Simultaneous AM-FM and tanð Imaging, T. Mehr, A. Moshar, R. Proksch, I. Revenko, N. Geisse, S. Hohlbauch, D. Walters, J. Cleveland, J. Bemis, C. Callahan, D. Beck, Asylum Research

Frequency-Modulated (FM) is a powerful, quantitative technique for mapping interaction forces between an oscillating tip and sample. Since FM-AFM typically requires the use of three feedback loops, one ongoing challenge has been stable and cross-talk free operation. Amplitudemodulated Atomic Force Microscopy (AM-AFM), also known as tapping mode, is a proven, reliable and gentle imaging method with wide spread applications. Recently, the phase signal of the first resonant mode has been recast in terms of the tip-sample loss tangent.[1] This allows quantitative imaging of a response term that includes both the dissipated and stored energy of the tip sample interaction. Combining AM and FM imaging allows reaping the benefits of both techniques.[2] Because the feedback loops are decoupled, operation is more robust and simple than conventional FM imaging. In this mode, the topographic feedback is based on the AM signal of the first cantilever resonance while the second resonance drive is frequency modulated. The FM image returns a quantitative value of the frequency shift that in turn depends on the sample stiffness and can be applied to a variety of physical models. We will present results on a wide variety of materials as well as discussing quantitative separation of the elastic and dissipative components of the tip-sample interactions.[3]

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5:40pm SP+AS+BI+ET+MI+TF-WeA12 Simultaneous Scanning Tunneling and Atomic Force Microscopy with Subatomic Spatial Resolution, *FJ. Giessibl*, University of Regensburg, Germany

Frequency-modulation AFM can be combined with scanning tunneling microscopy, yielding a simultaneous data set for current and average force gradient. Ternes et al. [1] have shown that for some metallic contacts, force and current are proportional. The interaction of a tungsten tip with a CO molecule adsorbed on Cu(111), however, yields a much different symmetry and distance dependence of tunneling current and force [2]. The tunneling current yields a gaussian dip over the CO molecule, while the forces show a

strong angular dependence with force fields that vary strongly by distance and angle within the extent of the single front atom, displaying subatomic variations. While the simultaneous acquisition of current and force can reveal new information about the atomic and electronic structure of matter, the tunneling current can modify the atomic forces. This "phantom force" [3,4], a modification of the electrostatic attraction between tip and sample, originates in an alteration of the effective potential difference between tip and sample caused by strongly localized voltage drop induced by the tunneling current. The talk discusses the potential of combined STM/AFM as well as the challenges, in particular with respect to tip preparation and characterization.

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Thin Film Room: 10 - Session TF+MI-WeA

Thin Films for Memory and Data Storage Moderator: S. Gupta, The University of Alabama

2:00pm TF+MI-WeA1 Spin Transport Properties and Applications in Magnetic Multilayers, *R.H. Victora*, *S.H. Hernandez*, *T. Qu*, University of Minnesota INVITED

Since the discovery of giant magnetoresistance (GMR) in 1988, spin transport has rapidly evolved as a research area examining effects such as Current Perpendicular to Plane (CPP) GMR and spin torque transfer (STT). Giant Magnetoresistance is caused by spin-dependent scattering. High electrical resistance (RAP) is measured for antiparallel magnetizations of adjacent layers, while low resistance (RP) is measured for parallel magnetizations. CPP GMR shows an advantage in MR ratio $((R_{AP}-R_P)/R_P)$, because all electrons must pass through all layers. This geometry is widely used as the reader in high areal magnetic recording, where it is likely that the current non-magnetic insulator will ultimately be replaced by a metallic layer in order to limit resistance. The reciprocal effect, STT, occurs when an electric current passes through a pinned ferromagnetic layer and the angular momentum (magnetic moment) is transferred to a neighboring free magnetic layer. The magnetization in the free layer may stably oscillate or may achieve a collinear state to the pinned layer. Magnetization switching with the help of a current has been proposed as potential magnetoresistive random access memory (MRAM). However, the mechanism of spin transport is not fully understood for these effects.

We consider multiple reflections between the interfaces of the adjacent magnetic layers. If the ferromagnetic material is not 100% polarized, electrons with different polarizations are not perfectly transmitted or reflected. We show that reflections, although typically neglected, strongly affect the spin transport properties. They explain¹ the experimentally observed nonlinearity of GMR dependence on $\beta = \cos^2(\theta/2)$ (θ is the angle between the magnetizations of the fixed and free layers). Also the spin torque is decreased² by the reflection. The more orders of reflection we include in the spin torque, the more critical current is needed to switch the magnetization state. The spin torque oscillator (STO) is an attractive replacement for current microwave devices owing to its very small (nanoscale) size. However, a single STO does not provide sufficient power for many applications. An array of oscillators in series or parallel has been proposed to generate more power. The problem is to phase lock the nonuniform oscillators. We calculate the power spectrum of serial oscillators. We show that the oscillators' could be closely synchronized by a feedback ac current, even at room temperature.

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2:40pm TF+MI-WeA3 Ta Seeded Ultrathin Free Layer for Fully Perpendicular Magnetic Tunnel Junctions, A. Singh, A. Natarajarathinam, B.D. Clark, S. Gupta, The University of Alabama

Studies of the effect of seed and capping layers on CoFeB free layers of magnetic tunnel junctions (MTJ's) originated from reports (1) of the crystallization of the CoFeB through diffusion of the B into the cap, as well as inducing an interfacial perpendicular magnetic anisotropy in the free layer (2, 3). We have also seen thatCoFeB can be made perpendicular[3, 4] with seed layers of certain materials, such as Ta and Ru. We deposited Ta and Ru seed layers with the following stack structure: (Ta/Ru/Hf/Zr) 2/ [tCoFeBx]/MgO 0.9/TaN5 nm. The thickness of CoFeB, tCoFeB, was varied between 0.8 to 1.4 nm. Samples with the Ta seed layer showed

higher perpendicular anisotropy than that of Ru, Hf and Zr because of the B diffusion into Ta after annealing. At tCoFeB = 1nm, high perpendicular anisotropy was seen, with anisotropy energy density Kut = 0.24 erg/cm2. The optimized Ta-seeded CoFeB was used as the free layer in a fully perpendicular MTJ stack with a Co/Pd multilayer synthetic antiferromagnet pinned layer[5]. These MTJ stackswere then patterned into devices with photolithography and planarized at each step of fabrication with a novel sputtered aluminum oxide passivation layer. After fabrication, these devices were subjected to a variety of annealing conditions: a) furnace annealed with a field of 0.5T applied in the plane of the sample at 1500C for 2 hours. b) rapid thermally annealed (RTA) at 3500C, 4000C and 5000C for various time periods. Magnetometry of the minor loops indicated that, as the RTA time was increased at each temperature, the free layer became fully perpendicular at 8 minutes and then went in-plane with longer annealing times of 12 minutes. These results matched closely with the transport measurements.Increase of annealing time improved the tunneling magnetoresistance (TMR) to a maximum of 50% at room temperature (nearly 60% at 4.2K). Further increase in annealing time degraded the TMR at all temperatures tested. Thus for the first time, we have found that magnetometry on the free layer of fully perpendicular magnetic tunnel junctions (pMTJ) can be used to optimize the annealing conditions.

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3:00pm TF+MI-WeA4 Epitaxial Fe_{38.5}Pd_{61.5} Films Grown by Pulsed Laser Deposition: Structure and Properties, *M.A. Steiner*, *R.B. Comes*, *J.A. Floro, W.A. Soffa, J.M. Fitz-Gerald*, University of Virginia

Thin films of 3d-4d/5d metallic alloys such as Fe-Pt, Co-Pt, and Fe-Pd are of technological interest due to their ordered L1₀ tetragonal phase which exhibits high magnetocrystalline anisotropy comparable to that of 3d-4f rare earth magnets. A combination of hard magnetic properties with ductility and corrosion resistance makes this family of alloys ideal for applications including micro-electro-mechanical systems and ultra-high-density magnetic storage. These alloys are known to develop unique microstructures, including a novel strain-induced chessboard eutectoid microstructure featuring exchange coupling effects that has been found between the hard L1₀ and soft L1₂ magnetic phases of the Co-Pt system. Within this class of materials, Fe-Pd alloys possess a somewhat lower magnetocrystalline anisotropy compared to Co-Pt and Fe-Pt, but the Fe-Pd phase diagram showing considerably lower order-disorder transition temperatures renders them well-suited for nanostructured magnetic applications and study.

Epitaxial films of Fe_{38.5}Pd_{61.5} at the L1₂-L1₀ eutectoid composition have been grown on MgO 001 oriented substrates by pulsed laser deposition. These films exhibit atomic ordering with increasing temperature, transitioning from the disordered A1 (FCC) phase to the ordered L1₂ phase. Fe_{38.5}Pd_{61.5} films grown at 550°C have been found to possess a two-phase microstructure of prismatic 50-100 nm disordered A1 secondary phases with 110 oriented facets embedded within an ordered L1₂ matrix. These secondary phases exhibit single domain magnetic axis rotation, while the easy magnetic axis of the ordered L1₂ matrix lies in plane due to strain induced by epitaxy. The growth these two-phase films has been studied as a function of deposition time. The films grown in this study were characterized by x-ray diffraction, vibrating sample magnetometry, atomic and magnetic force microscopy, and high resolution scanning electron microscopy.

Thursday Morning, November 1, 2012

Magnetic Interfaces and Nanostructures Room: 6 - Session MI+SP+AS-ThM

Emerging Probes in Magnetic Imaging, Reflectometry and Characterization

Moderator: Z. Gai, Oak Ridge National Laboratory, V. Lauter, Oak Ridge National Laboratory

8:00am MI+SP+AS-ThM1 Toward Microscopy with Direct Chemical and Magnetic Contrast at the Atomic Level, V. Rose, Argonne National Laboratory INVITED

In this talk we will discuss the development of a novel high-resolution microscopy technique for imaging of nanoscale materials with chemical, electronic, and magnetic contrast. It will combine the sub-nanometer spatial resolution of scanning tunneling microscopy (STM) with the chemical, electronic, and magnetic sensitivity of synchrotron radiation. [1] Drawing upon experience from a prototype that has been developed to demonstrate general feasibility, current work has the goal to drastically increase the spatial resolution of existing state-of-the-art x-ray microscopy from only tens of nanometers down to atomic resolution. The technique will enable fundamentally new methods of characterization, which will be applied to the study of energy materials and nanoscale magnetic systems. A better understanding of these phenomena at the nanoscale has great potential to improve the conversion efficiency of quantum energy devices and lead to advances in future data storage applications. The combination of the high spatial resolution of STM with the energy selectivity afforded by x-ray absorption spectroscopy provides a powerful analytical tool.

Work at the Advanced Photon Source, the Center for Nanoscale Materials, and the Electron Microscopy Center was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract DE-AC02-06CH11357.

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8:40am MI+SP+AS-ThM3 Effect of Sub-Micrometer Scale Magnetic Inhomogeneity on the Magnetoelectric Coupling in Manganites, A. Biswas, University of Florida INVITED

The conventional magnetoelectric (ME) coupling in multiferroics is defined as the effect of a magnetic/electric field on the electricpolarization/magnetization. However, the strength of the ME coupling is usually small. Our recent results have revealed methods for significantly increasing the ME coupling in perovskite manganites and can be summarized in two broad categories: (1) in the phase separated manganite (La_{1-y}Pr_y)_{1-x}Ca_xMnO₃ (LPCMO), we have discovered that anisotropic strain leads to a fluid-like ferromagnetic material which can be manipulated using an electric field leading to an unconventional ME coupling [1,2] and (2) an ME coupling in BiMnO₃ (BMO) thin films which is about 30 times larger than previously observed in single phase multiferroics [3]. I will discuss the origin of the ME coupling in both multiferroic and phase-separated oxides and relate it to inhomogeneous magnetic properties of the thin films, measured using techniques such as low temperature scanning probe microscopy, spin-polarized neutron reflectometry, and strain dependent electric polarization. Acknowledgement: NSF DMR-0804452

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9:20am MI+SP+AS-ThM5 Impact of Interfacial Magnetism on Magnetocaloric Properties of Thin Film Heterostructures, C.W. Miller, University of South Florida INVITED

In an effort to understand the impact of nanostructuring on the magnetocaloric effect, we have grown and studied gadolinium in $W(5nm)/Gd(30nm)/W(5nm)]_8$ heterostructures. The entropy change associated with the second-order magnetic phase transition was determined from the isothermal magnetization for numerous temperatures and the appropriate Maxwell relation. The entropy change peaks at a temperature of 284 K with a value of approximately 3.4 J/kg K for 30 kOe field change; the full width at half max of the entropy change peak is about 70 K, significantly wider than that of bulk Gd under similar conditions. The relative cooling power of this nanoscale system is about 240 J/kg,

somewhat lower than that of bulk Gd (410 J/kg). Polarized neutron reflectometry was used to determine the depth profile of the magnetic moment per Gd atom, m_{Gd} . Despite sharp interfaces observed by transmission electron microscopy, m_{Gd} is systematically suppressed near the Gd-W interfaces. Because the peak magnetic entropy change is proportional to $m^{2/3}$, the maximum achievable magnetocaloric effect in Gd-W heterostructures is reduced. By extension, our results suggest that creating materials with Gd-ferromagnet interfaces may increase the m_{Gd} relative to the bulk, leading to enhanced magnetocaloric properties. Together, these observations suggest that nanostructuring may be a promising route to tailoring the magnetocaloric response of materials.

Supported by AFOSR and NSF.

10:40am **MI+SP+AS-ThM9 Polarized Neutron Reflectometry on Exchange Biased Thin Films,** *K. Temst*, KU Leuven, Belgium **INVITED** Polarized neutron reflectivity has established itself as an important tool in the study of magnetic thin film systems. It provides a high-resolution magnetic depth profile and it offers vectorial probing of the magnetization. In recent years polarized neutron reflectivity has played an influential role in elucidating the magnetic structure of exchange bias systems, i.e. structures in which a ferromagnetic layer is coupled to an antferromagnetic layer. Exchange bias leads to a remarkable shift of the hysteresis loop, an increase in coercivity, and offen a pronounced asymmetry of the hysteresis loop shape as wellas a complex magnetic history. With this contribution we will take a closer look at two such exchange bias systems and highlight the role of polarized neutron reflectivity.

As a first model system, the archetypal exchange bias system Co/CoO will be highlighted. The antiferromagnetic CoO layer is prepared by oxidizing the surface of a Co thin film, by exposing it to a reduced oxygen atmosphere. We will review the properties of exchange bias in surfaceoxidized Co thin films, with the emphasis on the asymmetry of the magnetization reversal mechanism and the training effect. We will also discuss how the training effect can be (partially) restored by applying a magnetic field perpendicular to the initial cooling field direction. Recently we explored an alternative way to establish exchange bias between Co and CoO: rather than creating the antiferromagnetic CoO layer by oxidizing a metallic Co layer, the antiferromagnetic CoO is produced by implantation of oxygen ions into a Co layer. Polarized neutron reflectivity (PNR) is used to determine the magnetic depth profile and to probe the magnetization reversal mechanism. Simultaneously with the PNR measurements, in situ anisotropic magnetoresistance measurements were carried out.

The second example is a ferromagnet/antiferromagnet FePt/FePt₃ bilayer in which complementary use is made of polarized neutron reflectivity (for studying the magnetic depth profile in the ferromagnetic layer) and nuclear resonant scattering of synchrotron x-rays (making use of the Mössbauer effect) to probe the antiferromagnetic FePt3 layer. Below the Néel temperature, antiferromagnetic order appears in the FePt₃ layer with a spin wavevector pointing along the [100] axis. A net magnetization of the FePt₃, which increases towards the FePt/FePt₃ interface is found.

This work was supported by the Fund for Scientific Research-Flanders (FWO), the KULeuven Concerted Research Action program (GOA/09/006), the Belgian Interuniversity Attraction Poles research programs (IAP P6/42), and the KULeuven BOF (CREA/07/005) program.

11:20am MI+SP+AS-ThM11 Soft X-ray Microscopy to Study Complexity, Stochasticity and Functionality in Magnetic Nanostructures, *P. Fischer*, *M.-Y. Im*, Lawrence Berkeley National Lab, *S.-K. Kim*, Seoul National University, Republic of Korea

Research in magnetism is motivated by the scientific curiosity to understand and control spins on a nanoscale and thus to meet future challenges in terms of speed, size and energy efficiency of spin driven technologies. Imaging magnetic structures and their fast dynamics down to fundamental magnetic length and time scales with elemental sensitivity in emerging multi-element and nanostructured materials is highly desirable. Magnetic soft X-ray microscopy is a unique analytical technique combining X-ray magnetic circular dichroism (X-MCD) as element specific magnetic contrast mechanism with high spatial and temporal resolution [1]. Our approach is to use Fresnel zone plates as X-ray optical elements providing a spatial resolution down to currently 10nm [2] thus reaching out into fundamental magnetic length scales such as magnetic exchange lengths. The large field of view allows to investigate both the complexity, but also the stochasticity of magnetic processes, such as nucleation or reversal. Utilizing the inherent time structure of current synchrotron sources fast magnetization dynamics such as current induced wall and vortex dynamics in ferromagnetic elements can be performed with a stroboscopic pump-probe scheme with 70ps time resolution, limited by the lengths of the electron bunches.

We will present studies of magnetic vortex structures, where we found a stochastic character in the nucleation process, which can be described within a symmetry breaking DM interaction [3]. We will also present time resolved studies of dipolar coupled magnetic vortices, where we find an efficient energy transfer mechanisml, which can be used for novel magnetic logic elements [4].

This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DE-AC02-05-CH11231.

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11:40am MI+SP+AS-ThM12 Elemental and Magnetic Contrast using X-ray Excited Luminescence Microscopy, R.A. Rosenberg, S. Zohar, D. Keavney, Argonne National Laboratory, A. Mascarenhas, M. Steiner, National Renewable Energy Laboatory, D. Rosenmann, R.S. Divan, Argonne National Laboratory

We have developed an imaging technique based on x-ray excited luminescence microscopy (XELM), that will enable elemental and magnetic specific imaging of a wide range of materials such as those used in solar cells, magnetic materials, spintronic devices, ferroelectrics, and solid-state lighting. This new scientific tool utilizes the benefits of pulsed, polarized, tunable synchrotron radiation excitation with microscopic detection of the resulting optical emission. A unique offshoot of the microscope is the ability to perform element specific magnetic microscopy of micron-sized features or domains in magnetic fields. X-rays transmitted through thin films are attenuated and the resultant absorption spectrum can be determined by changes in the substrate luminescence. Since many substrates, such as SrTiO3 and GaAs, used in thin film growth have intense optical emission, this tool should impact many materials where photoelectron emission microscopy (PEEM) cannot be performed since it is not useable on insulating materials or if magnetic or electric fields are required. This approach will be especially useful at low temperatures where luminescence yields are highest, and PEEM has difficulties. In this presentation we will present some initial results from the microscope on some prototype solar cell materials and lithographically patterned Permalloy/GaAs and Permalloy/Cu/Co/GaAs samples. The results demonstrate the potential of XELM for elemental and magnetic specific imaging.

This work was performed at the Center for Nanoscale Materials and the Advanced Photon Source. It was supported by the U.S. Department of Energy, Office of Science and Office of Basic Energy Sciences under the contract number DE-AC02-06CH11357 and by the Department of Energy, Energy Efficiency and Renewable Energy, Solid State Lighting Program.

Thursday Afternoon, November 1, 2012

Electronic Materials and Processing Room: 9 - Session EM+MI-ThA

Semiconductor Heterostructures II + Heusler Alloys

Moderator: J.E. Ayers, University of Connecticut, B.D. Schultz, University of California, Santa Barbara

2:00pm EM+MI-ThA1 Dislocation Compensation in Ungraded ZnS_ySe_{1-y}/GaAs (001) Heterostructures, *T.M. Kujofsa*, *J.E. Ayers*, University of Connecticut

Control of strain and dislocation dynamics are important in determining the performance and reliability of semiconductor devices such as light-emitting diodes and photo-detectors. Experimental studies of ZnS_ySe_{1-y} /GaAs (001) heterostructures show that a dislocation compensation mechanism is active in structures involving abrupt interfaces. This mechanism involves the bending over of threading dislocations associated with misfit segments of one sense by misfit dislocations having the opposite sense, and it allows removal of threading dislocations from device structures.

Semiconductor device structures may be designed to take advantage of the dislocation compensation with the aid of a dislocation dynamics model accounting for misfit-threading interactions. To develop such a model we studied strain relaxation in ZnSe/GaAs (001) and ZnSySe_{1-y} /GaAs (001) heterostructures to determine the kinetic material parameters associated with dislocation glide and multiplication. Based on these results and by including misfit-threading interactions we developed a dislocation dynamics model which predicts dislocation compensation in arbitrary ZnSySe_{1-y}/GaAs (001) heterostructures.

Whereas our previous experimental work involved graded structures, this work focuses on the study of theoretical heterostructures comprising a device layer (DL) of ZnS_ySe_{1-y} on a ungraded buffer layer (BL) of ZnS_ySe_{1-y} deposited on a GaAs (001) substrate. We show that for a given device layer thickness and compositional change at the buffer-device layer interface there exists an optimum thickness of the ungraded buffer layer where the mobile threading dislocation density can be removed entirely. The optimum buffer layer thickness decreases monotonically with the compositional difference between buffer and device layer.

2:20pm EM+MI-ThA2 Dynamical X-ray Diffraction from Semiconductor Heterostructures with Asymmetrical Dislocation Densities, P.B. Rago, J.E. Ayers, University of Connecticut

We extend the dynamical theory of Bragg x-ray diffraction to include asymmetrical dislocation densities on the two types of active slip systems in zinc blende semiconductor heterostructures with (001) orientation. In such structures the dislocations exist in eight active slip systems of two basic types distinguished by the orientation of their misfit segments, which are oriented along either the [1-10] or [110] direction. Variation of the incident x-ray beam azimuth results in a change in the shape of the diffraction profile if the two types of slip systems exhibit an asymmetry in dislocation densities. Our work allows simulation of the x-ray diffraction profile of an arbitrary zinc blende semiconductor heterostructure, and through comparison to experimentally measured data, the two dislocation densities of an experimentally measured sample can be extracted. In this work we have demonstrated use of the model by applying it to the ZnSe/GaAs (001) and HgCdTe/CdTe (001) material systems.

3:40pm EM+MI-ThA6 Epitaxial Growth and Electronic Bandstructure of the Semiconducting Half Heusler Compound CoTiSb, J. Kawasaki, University of California Santa Barbara, L. Johansson, M. Hjort, R. Timm, Lund University, Sweden, B. Shojaei, University of California Santa Barbara, A. Mikkelsen, Lund University, Sweden, B.D. Schultz, C. Palmstrom, University of California Santa Barbara INVITED The Heusler compounds are an exciting class of intermetallics due to their ability to adopt a wide range of tuneable electrical and magnetic properties. These properties include ferromagnetism, paramagnetism, half-metallic ferromagnetism, large thermoelectric figures of merit, and both semiconducting and metallic behaviour. Additionally, some of the semiconducting Half Heuslers have been theoretically proposed be topological insulators, making the Heusler compounds a promising system for multifunctional heterostructure devices. However, due to challenges in controlling defects and stoichiometry, little is known about the experimental band structure of the semiconducting Half Heuslers. We demonstrate the epitaxial growth of the Half Heusler compound CoTiSb by molecular beam epitaxy. Samples consist of an InP (001) substrate, lattice matched In_xAl₁. xAs buffer layer, and CoTiSb layer. The films are single crystalline and of high structural quality, as measured in situ by reflection high energy electron diffraction (RHEED) and scanning tunnelling microscopy (STM) and ex situ by X-ray diffraction (XRD), with an out of plane lattice mismatch of less than 0.5%. For growth temperatures of less than 400°C the films grow in a layer-by-layer mode as demonstrated by RHEED intensity oscillations. Under stoichiometric growth conditions the films have a (2x1) surface reconstruction and for Sb-rich conditions the films have a (1x1) reconstruction. Electrical transport measurements show the resistivity of the films decreases as a function of temperature down to 10K, consistent with semiconducting behaviour, and using tunnelling differential conductance spectroscopy (dI/dV) we measure a band gap on the order of 160 meV. However, this band gap is much smaller than the value of 1.0 eV predicted by density functional theory. Angle resolved photoemission spectroscopy (ARPES) measurements were also performed at the MAX-Lab synchrotron facility in Lund, Sweden. A protective Sb capping and decapping scheme was developed to maintain the surface quality of the films as the samples are transported to the characterization facility and exposed to air. The structural, chemical, and electrical properties of the single crystal CoTiSb films will be presented to provide insights into the band structure of the semiconducting Half Heuslers. This work was supported in part by the Office of Naval Research and the National Science Foundation.

4:20pm EM+MI-ThA8 Application of Magnetic Heusler Alloys to All-Metal Sensors for Ultrahigh-Density Magnetic Recording, J.R. Childress, HGST San Jose Research Center INVITED Magnetic Heusler allovs are attractive materials for a number of applications in spintronics due to their potential high spin-polarization at the Fermi level, advantageous for spin-injection experiments and magnetoresistive devices. In the magnetic recording heads used in today's hard-disk drives (HDD's), the magnetoresistive thin-film sensors are multilayer spin-valves which operate in the current-perpendicular-to-filmplane (CPP) geometry, and rely on the spin-filtering properties of ultrathin MgO tunnel barriers (junction resistance < 1 Ohm-micron²) to achieve large tunnel-magnetoresistance (TMR) values using standard CoFe and CoFeB magnetic alloys as electrodes. Sensors with lower resistance (and thus lower-noise) are continuously required as sensor dimensions are reduced to keep up with the increased areal density of recorded data (approaching 1 Tb/in²). Intrinsically, an all-metal sensor can operate similarly to TMR sensors and will be able to achieve much lower resistances (~ 0.05 Ohmmicron²) and lower noise, but also requires a relatively large giant magnetoresistance (GMR) ratio to achieve sufficiently large signal to noise ratios (SNR). A number of Co-based full-Heusler alloys have the required magnetization, high T_{Curie} and a predicted half-metallic behavior at low temperatures, and are therefore of interest for this application. But while the high spin-polarization in these Heusler alloys can significantly increase the GMR signal, integrating these materials in recording head sensors is a challenge due to their complex crystalline structure which typically requires high-temperature processing, and strong sensitivity to compositional disorder. In addition, the high polarization and low magnetic damping observed in these materials results in a high sensitivity to spin-torque excitations which limits the maximum allowable bias voltage, and is also a source of noise which limits the signal to noise (SNR) ratio. The geometrical, thermal, and magnetic constraints which influence the integration of Heusler alloys in magnetic recording head sensors will be presented, along with some examples of materials characterization and multilayer stack optimization required to improve the properties and robustness of the devices. It is found that practical spin-valves with Heusler alloy-based magnetic layers can be fabricated with CPP-GMR ratios which can be increased to >10%, more than 2x larger than for conventional ferromagnetic alloys. The outlook for applicability of such sensors to magnetic recording at high densities > 1 Tb/in² will be discussed.

5:00pm EM+MI-ThA10 Growth of Epitaxial Co₂MnSi/MgO/Co₂MnSi Magnetic Tunnel Junctions by Molecular Beam Epitaxy, *S. Patel, A. Kozhanov, B.D. Schultz, C. Palmstrøm*, University of California, Santa Barbara

Epitaxial magnetic tunnel junctions (MTJs) have the potential to be used as low-energy non-volatile random access memory. The use of half metallic ferromagnets as electrodes has drawn great interest due to the predicted 100% spin polarization at the Fermi level. Co2MnSi is predicted to be halfmetallic[1], with a Curie temperature of 985K [2], and is a strong candidate for use in magnetic random access memory devices. These devices, however, are highly sensitive to interfacial and bulk disorder, which may result in the loss of a minority spin gap [3]. Therefore it is critical to understand the fundamental properties of the Heusler alloy films and correlate these properties with device performance. We have successfully grown highly-ordered, epitaxial Co2MnSi(001) films by molecular beam epitaxy (MBE) using a "seeded growth" technique to form a crystalline seed layer on various substrates, including MgO (001) and a Sc0.3Er0.7As lattice-matched diffusion barrier layer on GaAs (001). The lattice mismatch between GaAs and Co2MnSi is only -0.06% and x-ray diffraction of the MBE grown thin films show the two are nearly lattice matched. These films also have relatively smooth surfaces and coercivities down to 4 oersteds for stoichiometric films. Composition is also found to play a large role in the magnetic properties of the films. Off-stoichiometry films display lower saturation magnetization as well as higher coercivities. We have subsequently been able to grow epitaxial MTJ heterostructures of Co2MnSi/MgO/Co2MnSi with different switching fields for the top and bottom electrodes. We have characterized the structure of each layer and interfaces with reflection high-energy electron diffraction (RHEED), lowenergy electron diffraction (LEED), scanning tunneling microscopy (STM) and cross-sectional transmission electron microscopy (XTEM) and the corresponding magnetic properties using vibrating sample magnetometry (VSM) and a superconducting quantum interference device (SQUID) to better understand the fundamental properties of these epitaxial heterostructures. This work was supported in part by the Semiconductor Research Corporation under award number 2011-IN-2153.

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5:20pm EM+MI-ThA11 Fabrication of Highly Ordered Co₂FeAl Thin Films by Reactive Ion Beam Deposition for Spintronic Devices, Y.S. Cui, University of Virginia, S. Schäfer, T. Mewes, University of Alabama, M. Osofsky, Naval Research Laboratory, J.W. Lu, S.A. Wolf, University of Virginia

Co₂FeAl (CFA) is a full Heusler alloy that has potentially very low damping parameter and high spin polarization, highly desired for spintronic devices such as magnetic tunnel junctions and spin valves. CFA with B2-type chemical ordering has shown an extremely low Gilbert damping parameter among the Heusler alloys, which facilitates spin dynamics such as spin current driven magnetization switching. A large tunnel magnetoresistance (TMR) has been reported in B2-CFA based magnetic tunnel junctions, which is ascribed to its intrinsic high spin polarization efficiency. The high spin polarization efficiency originates from the half-metal gap in some of its energy bands with certain symmetry. It was predicted by theory that both low damping parameter and high spin polarization can only be achieved with a high chemical ordering existing in the CFA crystal structure. We will present the synthesis of high quality CFA thin films, prepared by a novel deposition technology, Reactive Biased Target Ion Beam Deposition (RBTIBD). The surface roughness (RMS) was observed as low as 0.14 nm. It was determined that CFA thin films grew on MgO(001) epitaxially along both in-plane and out-of-plane directions with a B2-type chemical ordering, according to the results obtained in XRD and TEM. The chemical ordering can be significantly improved by properly choosing the post annealing parameters. The ferromagnetic resonance (FMR) measurements suggested an extremely small damping parameter (~0.002). The damping parameter was strongly correlated with the chemical ordering of B2 structure. In addition, the impact of chemical ordering on the spin polarization efficiency of CFA films based on PCAR measurements will be discussed.

Thursday Afternoon Poster Sessions

Magnetic Interfaces and Nanostructures Room: Central Hall - Session MI-ThP

Magnetic Interfaces and Nanostructures Poster Session

MI-ThP1 Magnetic Properties of Ferromagnetic-Antiferromagnetic Bi-Layers with Different Spin Configuration, W. Kim, Korea Research Institute of Standards and Science (KRISS), G.-E. Yang, Chungnam National University, Korea, C. Hwang, Korea Research Institute of Standards and Science (KRISS), E. Cho, Chungnam National University, Korea

We investigated the effect of different spin direction of antiferromagnetic(AFM) layer on the magnetic properties of ferromagnetic(FM) layer in Fe-NiO and Fe-CoO bi-layer systems. For Fe-NiO system, we prepared successfully Fe/NiO/Ag(001) and Fe/NiO/MgO(001) systems on a single MgO(001) substrate. We examined magnetic properties of the bi-layer system using the surface magnetic optical Kerr effect(SMOKE) and X-ray magnetic linear dichroism(XMLD). From SMOKE measurement we observed the coercivity enhancement due to the set-up of AFM order of NiO films in both of the Fe/NiO/MgO(001) and Fe/NiO/Ag/MgO(001) system. The most remarkable results in our observation is that the coercivity enhancement of Fe/NiO/Ag/MgO(001) is much larger than that of Fe/NiO/MgO(001). XMLD experiments confirmed the out-of-plane spin direction of NiO layers in Fe/NiO/MgO(001) and inplane spin-direction of NiO layers in Fe/NiO/Ag/MgO(001), and we concluded that the origin of large enhancement of coercivity is due to the strong parallel coupling between Fe layers and NiO layers. We also confirmed that this strong parallel coupling maintained across the thin Ag layer inserted between Fe and NiO layers. With this Ag inserted Fe/NiO system, we could estimate the Neel temperature of the NiO layers. We also realized different spin configuration in Fe-CoO systems by growing CoO films on theAg(001) and MnO(001) surfaces. We observed much larger coercivity enhancement in Fe/CoO/Ag(001) than in Fe/CoO/MnO(001) below the Neel temperature of CoO films.

MI-ThP2 Spin Dynamics and Exchange Bias in Core-Shell Fe\γ-Fe₂O₃ Nanoparticles, S. Chandra, H. Khurshid, University of South Florida, W. Li, G.C. Hadjipanayis, University of Delaware, M.H. Phan, H. Srikanth, University of South Florida

Exchange bias in core-shell nanoparticles has been an area of intense research. While several research efforts have been devoted in understanding the role of interfacial spins in the nanoparticles that exhibit exchange bias, a clear understanding of the spin dynamics of the core and the shell remains to be investigated. A detailed study has been carried out on the magnetic properties of Fe/ γ -Fe2O3 core-shell structured nanoparticles synthesized by thermal decomposition method.Our focus is to understand the spin dynamics of the core and shell independently and their role in triggering exchange bias (EB) phenomenon. The nanoparticles exhibit memory effect and aging associated with a superspin glass state (SSG). We show that the energy barrier distribution shows two maxima that marks the freezing temperatures of the core and shell. Lastly, hysteresis measurements after field cooling reveal a strong EB indicated by a loop shift. The onset of EB is at 35 K when the ferromagnetic core is frozen and the moments in the ferrimagnetic shell begin to block resulting in enhanced exchange coupling.

MI-ThP4 Modeling-assisted Synthesis and Characterization of Epitaxial NiTiO₃ Films as New Multiferroics, *T. Varga*, *T.C. Droubay*, *M.E. Bowden*, *S.A. Chambers*, *B.C. Kabius*, *E. Apra*, *W.A. Shelton*, *V. Shutthanandan*, Pacific Northwest National Laboratory

In a search for new multiferroic materials where the direction of magnetization can be switched by an applied electric field, we have looked for materials in which polarization and magnetization are strongly coupled. Recent theory calculations predicted that the family of compounds MTiO₃ (M = Mn, Fe, Ni), in a certain polymorphic structure (acentric *R3c*), are promising candidates where a polar lattice distortion can induce weak ferromagnetism. Guided by these insights, a rhombohedral phase of Ni TiO₃ has been prepared in epitaxial thin film form, whose structure is of the predicted multiferroic. Preliminary physical property measurements suggest a Neel transition also consistent with the R3c structure and SHG imaging shows a polarized lattice. The synthesis of epitaxial NiTiO₃ films, their full structural characterization and physical property measurements along with our first-principles DFT calculations to predict the desired NiTiO₃ structure, its stability, and the effect of lattice strain on the growth are reported.

MI-ThP5 Nanomechanical Manipulation of the Anomalous Hall Effect in GaMnAs, J.H. Lee, M.L. Cho, Y.D. Park, Seoul National University, Republic of Korea

We show an explicit dependence of the anomalous Hall effect (AHE) as well as magnetic anisotropy (MA) on locally induced mechanical strains in low-temperature molecular beam epitaxy (LT-MBE) prepared GaMnAs. LT-MBE GaMnAs (001) epilayers were prepared on AlGaAs layer, which serves (1) to enhance compressive strain in GaMnAs during growth as well as (2) to act as a sacrificial layer. By selective nanopatterning and removal of the AlGaAs layer, we realise free-standing GaMnAs microbeams (along (110),(110), and (100) directions) with multiple lateral probes along the length of the microbeam. Due to the relaxation of the the compressive strain when released, GaMnAs microbeam mechanically buckles. By simultaneous measurements of ρ_{xx} and ρ_{xy} along the length of the buckled GaMnAs microbeam (1.4 K < T < 300 K), we probe both AHE and MA as functions of local strain. We find relatively small changes in MA while large suppression of AHE for regions along the microbeam experience the highest mechanical strain. We demonstrate the novelty of such interplay between mechanical strain and AHE by realising simple Hall crosses which mechanical state can be robustly read by the AHE signal - which correspondence between mechanical state and transport properties are well suited for a low-power, non-volatile memory elements. Furthermore, we demonstrate the applicability of above methods beyond GaMnAs to other material systems which are sensitive to small mechanical strains via strong spin-orbit interactions, namely topological insulator Bi2Se3.

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