Tuesday Afternoon, November 1, 2011

Graphene and Related Materials Focus Topic
Room: 208 - Session GR+MI-TuA

Graphene: Magnetic Properties and Spin-Dependent Phenomena

Moderator: A.C. Ferrari, University of Cambridge, UK

2:00pm **GR+MI-TuA1 Magnetic Impurities on Graphene**, ***K. Kern***, Max Planck Institute for Solid State Research, Germany **INVITED**

Hybrid systems consisting of transition metal (TM) atoms in contact with graphene are expected to show outstanding magnetic effects, from Kondo screening to long range ferromagnetism due to the large Fermi wavelength in graphene. First recent experimental evidence supports this scenario, however, little is known about the nature of the chemical interaction between TM atoms and graphene, which is the necessary starting point for any advanced application. Here we present recent X-ray Absorption Spectroscopy (XAS) and X-ray Magnetic Circular Dichroism (XMCD) experiments probing the electronic configuration and magnetism of Fe, Co and Ni impurities on graphite and various graphenes. We find a rich physical scenario with marked differences between graphite and silicon oxide supported graphene on one hand and few layer epitaxial graphene on the C-face of silicon carbide on the other hand.

2:40pm **GR+MI-TuA3 Electron Spin Transport in Exfoliated and Epitaxial Graphene Grown on SiC**, ***J. Abel***, *A. Matsubayashi, J.J. Garramone,* University at Albany, *C. Dimitrakopoulos, A. Grill, Sung,* IBM T.J. Watson Research Center, *V.P. LaBella*, University at Albany

Graphene is an ideal candidate for the transport channel in future spintronic devices due to its long spin lifetimes at room temperature. The long lifetime arises due to the small intrinsic spin orbit coupling and low hyper-fine interaction of the electron spins with the carbon nuclei. Non-local Hanle measurement devices were fabricated on epitaxially grown graphene on SiC, provided by IBM, and multi-layer exfoliated flakes. Spin injection and detection were achieved in these devices using cobalt nano-magnets directly deposited on the graphene. Spin precession was observed and the spin lifetimes for the epitaxial graphene were found to be comparable to those found in the exfoliated multi-layer flake. We will also present our measurements of spin relaxation as a function of temperature. The temperature dependence in the spin lifetime observed in the exfoliated flake show a coupling between the magnetic contacts and graphene channel. This is expected due to the lack of a tunnel barrier contact. The comparable spin relaxation times measured in epitaxial graphene fabricated with similar contacts and the multi-layer flake is believed to be caused by a large contact induced relaxation due to the contacts coupling with the graphene channel. The strong coupling effectively removes the spin from the channel.

3:00pm **GR+MI-TuA4 Landau Levels of Dirac Fermions Observed at Zero External Magnetic Fields on Modified Graphite by STS**, ***T. Kondo***, *D. Guo, T. Machida, T. Suzuki, K. Iwatake, S. Okada, J. Nakamura*, University of Tsukuba, Japan

Under the external magnetic field, carriers of graphene are quantized to show an unusual Landau level (LL) energy spectrum due to mass-less Dirac fermions (DFs).[1] The LL energies are not equally spaced and include a characteristic zero-energy state (the n = 0 LL) contrary to the case of normal metals or two-dimensional electron gases. As a result, anomalous quantum Hall effect of graphene has been observed.[2, 3] The quantization of the graphene carrier also occurs without external magnetic field if the appropriate strain is induced.[4,5]Here, we report spontaneous LLs formation of mass-less DFs on potassium intercalated graphite (K-Graphite) and nitrogen-doped graphite (N-Graphite) under zero external magnetic field with the use of scanning tunneling spectroscopy (STS). On the basis of the calculation with the density functional theory, the top-most graphene layer is found to be decoupled with the graphite due to the partial intercalation of potassium atom or nitrogen-doping on graphite. Partially decoupled graphene layer has a sufficient strain to generate the pseudo-magnetic field with about 280 T and 60 T for K-Graphite and N-Graphite, respectively, leading to the LLs formation on the top-most graphene layer on graphite.

1. A. H. Castro Neto et al., Rev. Mod. Phys. 81 (2009) 109.

2. K. S. Novoselov et al., Nat Phys. 2 (2006) 177.

3. K. S. Novoselov et al., Science. 306 (2004) 666.

4. F. Guinea et al., Nat Phys. 6 (2010) 30.

5. N. Levy et al., Science. 329 (2010) 544.

4:00pm **GR+MI-TuA7 Tunneling Spectroscopy of Adsorbed Iron Phthalocyanine on Epitaxial Graphene on SiC(0001)**, ***A.A. Sandin***, *D.B. Dougherty, J.E. Rowe*, North Carolina State University

Graphene may be an ideal material for spin field effect transistors because of its high charge carrier mobility and long spin relaxation times due to small spin-orbit coupling.[1] However, efficient spin injection into graphene requires overcoming conductivity mismatch through the use of tunnel barriers and/or spin filters.[2] It is possible that organic films can serve as tunnel barriers/spin filters with highly tailorable properties. In particular, metal phthalocyanines have recently been shown to exhibit spin dependent interfacial coupling on magnetic electrodes.[3] A study of the coupling and morphology of such molecules on graphene is a crucial first step to understand potential spin enhanced interfaces.

We deposit monolayer iron phthalocyanine (FePc) on both single layer and bilayer epitaxial graphene on the Si-terminated polar face of SiC, named SiC(0001). Scanning tunneling microscopy reveals an adsorbed molecular lattice periodicity of 1.8 nm, close to that of the graphene/SiC buffer layer corrugation periodicity. This lattice spacing is larger than that of FePc adsorbed on a graphite surface that shows a smaller spacing of ~1.4 nm. This implies a stronger interaction of the FePc with epitaxial graphene than expected and is possibly due to the modification of graphene by the SiC substrate. Tunneling spectroscopy has been used to study the occupied and unoccupied electronic states of the absorbed monolayer FePc. Broad unoccupied states indicate significant electronic coupling between the molecules and the graphene and suggest a promising future for molecular strategies for spin injection.

*Supported by the NSF Center for Chemical Innovation: Center for Molecular Spintronics under CHE-0943975.

1. Y. G. Semenov, K. W. Kim and J. M. Zavada, Appl. Phys. Lett. 91 (15), 3 (2007).

2. W. Han, K. Pi, K. M. McCreary, Y. Li, J. J. I. Wong, A. G. Swartz and R. K. Kawakami, Phys. Rev. Lett. 105 (16), 4 (2010).

3. C. Iacovita, M. V. Rastei, B. W. Heinrich, T. Brumme, J. Kortus, L. Limot and J. P. Bucher, Physical Review Letters 101 (11), 116602-116604 (2008).

4:20pm **GR+MI-TuA8 Atomic Scale Determination of the Bilayer Graphene Energy Gap**, ***S. Jung***, *N.N. Klimov, D.B. Newell, N.B. Zhitenev, J.A. Stroscio*, NIST

We have performed scanning tunneling spectroscopy measurements on a gated bilayer graphene device. In graphene bilayer, a potential asymmetry between the layers induces an energy gap in the electron spectrum. The formation of the energy gap is investigated as a function of carrier density and magnetic field. We found that in zero magnetic field, the reliable determination of the gap can be complicated because of disorder scattering. However, in the quantum Hall regime, the energy gap can be quantitatively determined by measuring the layer-polarized low index Landau levels.

Our scanning tunneling spectroscopy measurements reveal that the microscopic nature of the bilayer gap is very different from what was observed in previous macroscopic measurements or expected from current theoretical models. The potential asymmetry varies spatially in both magnitude and sign on a nanometer length scale, showing strong correlation with the disorder potential. This random pattern of alternating dipole fields is qualitatively consistent with the reduced disorder-induced density fluctuations in the top layer.

4:40pm **GR+MI-TuA9 Atomic, Electronic, and Magnetic Properties of Metal-Graphene Interfaces**, ***I.I. Oleynik***, *L. Adamska, Y. Lin,* University of South Florida, *A. Ross,* Saint Anselm College, *M. Batzill*, University of South Florida

Metal/graphene interfaces play an important role in both surface science studies of the epitaxial growth of graphene on metallic substrates, as well as in metal/graphene contacts in graphene nanoelectronic devices. We present results of first-principles density functional theory (DFT) investigations of structural, electronic, and magnetic properties for graphene/Ni(111) and graphene/Cu(111) interfaces relevant to experimental studies of graphene growth on metallic substrates. The favored interface geometries and binding sites for different interface configurations were identified. Additional adlayers of Ni and Cu were either adsorbed on top of the graphene/metal interface, or placed between the graphene and substrate to model processes of metal intercalation. It was also found that the interaction between graphene/Ni(111) and the top Cu adlayer is much weaker compared to that for a Ni adlayer. The atomic, electronic, and magnetic properties of these

interfaces, including induced magnetic moments in graphene/Ni(111), Ni/graphene/Ni(111) systems, are also discussed.

5:00pm **GR+MI-TuA10 Spin-Dependent Scattering from Gated Potential Obstacles in Graphene Systems**, ***M. Asmar***, *S. Ulloa*, Ohio University

We study the scattering of Dirac fermions in a sheet of graphene from potential obstacles created by external gates in the presence of both intrinsic and extrinsic spin-orbit (SO) interactions [1]. Obtaining analytical solutions in a real-space representation for the eigenvectors allows us to calculate the phase shifts generated by a finite-size obstacle in the presence of SO interactions [2]. From the phase shifts extracted from these solutions we can calculate the differential, total and transport cross sections. The knowledge of these quantities allows us to obtain the spin-flip and momentum relaxation times. The dependence of both relaxation times on the strength of the SO interaction was analyzed showing comparable relaxation times for relatively large values of energy, while displaying a big difference for small values of energy. The relaxation times of the injected electrons exhibit a number of resonances in energy associated with the structure of the scattering obstacle. In the presence of SO, new resonances appear at energies that depend on the strength of the SO interactions, and as such contain spectroscopic information on the system. It has been shown that the main scattering mechanism in graphene is due to strong defects [3]. Therefore, the analysis performed in our work can help understand the role of SO interactions in the scattering processes in these and related experiments.

[1] C. L. Kane and E. J. Mele, PRL 95, 226801 (2005).

[2] A. H. Castro Neto and F. Guinea, PRL 103, 026804 (2009).

[3] M. Monteverde, C. Ojeda-Aristizabal, R. Weil, K. Bennaceur, M. Ferrier, S. Gueron, C.Glattli, H. Bouchiat, J. N. Fuchs, and D. L. Maslov, PRL 104, 126801 (2010).

5:20pm **GR+MI-TuA11 Suppression of Weak-Localization Effect in Strained CVD –grown Graphene**, ***X. Miao***, *S. Tongay, M. Lemaitre, B.R. Appleton, A.F. Hebard*, University of Florida

We investigate the magnetic field and temperature-dependent transport properties of CVD-grown graphene subjected to different strains. The graphene is transferred to kapton substrates to which a blending force can be applied. In zero magnetic field, the prefactor to the logarithmic-in-temperature conductivity correction decreases by an approximate factor of 3 for strains as high as 0.6 %. There is also a concomitant decrease in diffusivity by a factor of 6. At 5 K we observe negative magnetoresistance for fields up to 0.5 Tesla followed by positive magnetoresistance at higher fields. We attribute the low field negative magnetoresistance to weak-localization and find that it is well described by theory. The strains resulting from the applied blending force inhibit the intervalley scattering more than an order of magnitude and decrease the phase coherence length, thereby leading to a suppression of weak-localization.

5:40pm **GR+MI-TuA12 Simulation of Electron-Ion Dynamics in Pristine and Functionalized Graphene in External Fields**, ***S. Bubin***, *K. Varga*, Vanderbilt University

In the framework of real-time real-space time-dependent density functional theory (TDDFT) we have studied coupled electron-ion dynamics in small fragments of graphene, graphane, and fluorinated graphene subjected to short (a few femtoseconds) intense laser pulses or irradiated by energetic ions. The goal of this study is to investigate the possibility of defect creation in graphene and desorption of hydrogen/fluorine from graphene surface. We will present the results of our simulations, discuss the mechanisms that take place, and identify the parameters of the laser or energetic ions necessary for those processes to occur.

Magnetic Interfaces and Nanostructures Division
Room: 105 - Session MI-WeM

Fundamental Problems in Magnetism

Moderator: C. Clavero, College of William and Mary

8:00am **MI-WeM1 Fundamental Problems in Magnetism**, ***W.H. Butler***, The University of Alabama **INVITED**

In this presentation, we shall attempt to describe the fundamental magnetic properties, the physics that controls and limits them and the practical implications of possible improvement. The most important fundamental properties of magnetic materials are Curie temperature, saturation magnetization, and magnetic anisotropy. The maximum Curie temperature (Co) and maximum saturation magnetization ($Fe_{65}Co_{35}$) at room temperature have not increased in a century. We shall discuss the reasons for this and speculate on the prospects that either may be increased. The magnetic anisotropy is somewhat less refractory. We shall discuss the prospects and implications of significant increases. Although higher room temperature saturation magnetization would be very useful, there would also be interesting applications for a magnetic material with very low magnetization, but very strong spin dependence of its transport properties. There are also interesting potential applications for insulating ferromagnets.

8:40am **MI-WeM3 Progress toward Understanding the Sign of Spin-Polarization at Interfaces in Organic Spin-Valves**, ***G.J. Szulczewski***, University of Alabama

In this talk I will present results from a systematic study to understand the role of LiF, Al_2O_3, and MgO tunnel barriers in organic spin-valves. The overall aim of this work is to better quantify the degree of spin-polarized electron injection and extraction at ferromagnetic metal/organic semiconductor interfaces. In general we find that spin-valves made with two ferromagnetic transition metals has a positive magnetoresistance. However, when one of the ferromagnetic metals is exchanged with $La_{0.67}Sr_{0.33}MnO_3$, the sign of the magnetoresistance is inverted. In addition the spin-polarized tunneling measurements the structural, electronic, and magnetic properties of these interfaces have been thoroughly investigated by cross-sectional transmission microscopy, photoelectron spectroscopy, and polarized neutron reflectometry. These results will be compared to other findings in the literature in order to summarize the current status of spin-polarized electron transport across organic semiconductor/insulator/ferromagnetic metal interfaces.

9:00am **MI-WeM4 Rational Design of New Spintronics Materials: From Topological Insulators and Spin Torque Applications**, ***C. Felser***, Johannes Gutenberg University Mainz, Germany **INVITED**

Heusler compounds are a remarkable class of intermetallic materials with 1:1:1 (often called Half-

Heusler) or 2:1:1 composition comprising more than 1500 members [1]. Today, more than a century after their discovery by Fritz Heusler, they are still a field of active research. New properties and potential fields of applications emerge constantly; the prediction of topological insulators is the most recent example [2]. Surprisingly, the properties of many Heusler compounds can easily be predicted by the valence electron count or within a rigid band approach. Their extremely flexible electronic structure offers a toolbox which allows the realization of demanded but apparently contradictory functionalities based on a virtual lab approach. The subgroup of more than 250 semiconductors is of high relevance for the development of novel materials for energy technologies. Their band gaps can readily be tuned from zero to 4 eV by changing the chemical composition. Thus, great interest has been attracted in the fields of thermoelectrics and topological insulator research. Ternary materials based on multifunctional properties, i.e. the combination of two or more functions such as superconductivity and topological edge states will revolutionize technological applications. The design scheme for topological insulstors from the view point of bands and bond will be presented.

The wide range of the multifunctional properties of Heusler compounds is reflected in extraordinary magneto-optical, magneto-electronic, and magneto-caloric properties. Tetragonal Heusler compounds Mn_2YZ as potential materials for STT applications can be easily designed by positioning the Fermi energy at the van Hove singularity in one of the spin channels [3]. A high calculated magnetic anisotropy energy (MAE) is the sufficient condition for a material with perpendicular magnetocrystalline anisotropy (PMA). Materials with saturation magnetizations of 0.2 – 4.0 μ_B, high Curie temperatures of 380 – 800 K, high spin polarizations, PMA, and required lattice constant matching with MgO can be realized with ferri- or ferromagnetic Heusler-related compounds. Such materials are strongly recommended for the spin transfer torque magnetic random access memory (STT-MRAM) data storage and the spin torque oscillators (STO) for telecommunication. Additionally the first spin gapless semiconductor is realized in Mn_2CoZ.

9:40am **MI-WeM6 Interfacial Effect on the Magnetic Properties of Core-Shell Co/Pt Supported Nanodots**, *P. Campigilo, N. Moreau, V. Repain,* ***C. Chacon***, Lab. Mat. et Phénomènes Quantiques, France, *H. Bulou, F. Scheurer,* Inst. de Phys. et Chimie des Mat. de Strasbourg, France, *P. Ohresser,* Synchrotron SOLEIL, France, *H. Magnan,* Service de Phy. et Chimie des Surfaces et Interfaces, France, *E. Fonda,* Synchrotron SOLEIL, France, *J. Lagoute, Y. Girard,* Lab. Mat. et Phénomènes Quantiques, France, *C. Goyhenex,* Inst. de Phys. et Chimie des Matériaux de Strasbourg, France, *S. Rousset*, Lab. Mat. et Phénomènes Quantiques, France

Core-shell nanoparticles have been receiving an increasing attention in order to practically employ magnetic clusters in devices [1]. The shell permits to protect the magnetism of the core, which readily oxidize in environmental conditions. Moreover, the shell can donate to the particle new chemico-physical functionalities which, combined with magnetism, permit to obtain multifunctional systems. Cobalt self-organized supported nanodots are promising candidates for applications as very high density magnetic recording media. However, it is necessary to improve the magnetic stability of such small nanostructures against thermal excitations. The capping with a non-magnetic metal of magnetic nanostructures induces different interfacial phenomena which together lead to a modification of the magnetic behavior of the system.

In the present work, the growth and the magnetism of Co/Pt core-shell have been studied. Pt has been deposited as over layer on Co self-organized on Au(111) template. The structural properties have been addressed by combining Scanning Tunneling Microscopy (*STM*) and Surface Extended X-ray Absorption Fine Structure (*SEXAFS*) measurements with molecular dynamics calculations. Magneto-Optic Kerr Effect (*MOKE*) and X-ray Magnetic Circular Dichroism (*XMCD*) have been coupled in order to identify the main magnetic phenomena acting at the Co/Pt interface. In the submonolayer regime, Pt forms metal rims around Co nanodots, and the Co magnetic anisotropy decreases. On the other hand, if more than one monolayer of Pt is deposited, the Co dots are completely covered and their magnetic anisotropy is enhanced. Furthermore, the Pt capping is found to have a minor effect of the cobalt magnetic moments. By changing the deposition conditions and by comparing the effect of Pt and Au capping [2], we identified three principal phenomena at the Co/Pt interface: inter-mixing, magnetoelasticity and band hybridization. Our results indicate that the principal one is band hybridization, which is responsible for the observed increasing of magnetic anisotropy. Intermixing and magnetoelasticity have rather the opposite effect and tend to decrease the magnetic anisotropy energy. The knowledge of the interplay between these different phenomena is fundamental in order to tune the magnetic properties of nanoparticles for precise applications, from data storage to biomedical research.

[1]A. Lu, E. Salabas, and F. Schüth, Angew. Chem. Int. Ed. 46, (2007) 1222.

[2] Y. Nahas, V. Repain, C. Chacon, Y. Girard, J. Lagoute, G. Rodary, J. Klein, S. Rousset, H. Bulou, and C. Goyhenex, Phys. Rev. Lett., 103 (2009) 067202.

10:40am **MI-WeM9 Spin-Split Bands in Non-Magnetic Systems**, ***E. Vescovo***, Brookhaven National Laboratory **INVITED**

For fundamental and technological reasons materials with a spin-split electronic band structure in proximity of the Fermi level are highly attractive. The possibility of separately manipulating the two spin channels introduces novel functional behaviors without counterpart in the corresponding spin-degenerate systems. A promising approach in this field consists in the exploitation of the spin-orbit interaction, which couples spin and orbital degrees of freedom. The Rashba interaction offers particularly interesting perspectives: at the surface of a crystalline material the breaking of the full translational symmetry gives rise to an effective (Rashba) electric field which splits in k-space the valence electrons with opposite spin orientations. For heavy elements, such as Bi, the Rashba interaction results in spin-polarized surface bands, detectable in angle-resolved photoemission experiments [1]. In this talk various cases of such systems will be presented. Bi-Ag(110) surface alloy allows to study the anisotropy of splitting induced by the anisotropic electric fields of the (110) – surface. The system Bi-Ag(111)/ Fe(110) provides direct evidence of the interplay between the

Rashba splitting of the Bi-Ag alloy and the ferromagnetic splitting of the Fe bands.

[1] Yu. M. Koroteev, G. Bihlmayer, J. E. Gayone, E. V. Chulkov, S. Blügel, P. M. Echenique, and Ph. Hofmann, Phys. Rev. Lett. 93, 046403 (2004); T. Hirahara, T. Nagao, I. Matsuda, G. Bihlmayer, E. V. Chulkov, Yu. M. Koroteev, P. M. Echenique, M. Saito, and S. Hasegawa, Phys. Rev. Lett. 97, 146803 (2006).

11:20am **MI-WeM11 Unoccupied Electron States in Rashba Systems Studied by Spin-Resolved Inverse Photoemission**, ***M. Donath***, *S.N.P. Wissing, A. Zumbülte, C. Eibl, A.B. Schmidt*, Muenster University, Germany

We present the first spin-resolved inverse-photoemission measurements of the unoccupied part of the Rashba-split surface state on Au(111). This Shockley-type state is considered as the prototype of a Rashba-split electron state on a metallic surface. The spin splitting of the occupied part of this state was first indicated by spin-integrated photoemission data [1]. This pioneering work was followed by a spin-resolved study, which directly proved the spin structure of the state [2].

Our study complements the information on the spin character by following the surface state into the unoccupied energy region. The state crosses the Fermi energy as a function of the wave vector parallel to the surface and finally leaves the bulk-band energy gap. Our spin-resolved inverse-photoemission experiment stands out from conventional systems thanks to an improved energy and **k** resolution [3]. Our data confirm the spin character of the surface state, as far as it does not overlap with bulk states. In addition, we show how the spin character is altered when the surface state becomes degenerate with bulk states.

Further Rashba systems with even larger spin splittings as well as topological insulators are currently investigated with our spin-resolved inverse-photoemission apparatus. We will provide a status report on our latest results.

[1] LaShell *et al.*, Phys. Rev. Lett. **77**, 3419 (1996)

[2] Hoesch *et al.*, Phys. Rev. B **69**, 241401(R) (2004)

[3] Budke *et al.*, Rev. Sci. Instrum. **78**, 083903 (2007)

11:40am **MI-WeM12 MBE Growth of Topological Insulator Bi_2Se_3 on Epitaxial Graphene on 6H-SiC(0001)**, ***Y. Liu****, *M. Weinert, L. Li*, University of Wisconsin-Milwaukee

In this work, we report results on the MBE growth of Bi2Se3, a prototypical topological insulator, on epitaxial graphene on 6H-SiC(0001). In situ scanning tunneling microscopy indicates spiral growth, characterized by atomically smooth terraces 10 to 50 nm in width, separated by steps of 1-2 quintuple-layers in height. X-ray diffraction shows only the (003) family of diffraction peaks with a full width at half maximum of 0.1 degree. Raman spectroscopy reveals two characteristic peaks at 130.21 and 171.48 cm-1, corresponding to the in-plane Eg2 and out-of-plane A1g2 vibrational modes, respectively. The close resemblance of the positions and line shapes of both these peaks to those of bulk Bi2Se3 attest to the very high quality of the film. These results and their impact on the properties of the topologically protected surface states of the Bi2Se3/graphene heterostructure will be presented at the meeting.

*Ying Liu applied for postdoctoral fellow award

Neutron Scattering Focus Topic
Room: 207 - Session NT+AS+MI-WeM

Applications of Neutron Scattering I
Moderator: V. Lauter, Oak Ridge National Laboratory

8:00am **NT+AS+MI-WeM1 A Deeper Look into Spintronic Material Systems with Neutrons and Synchrotron Radiation**, ***T. Brueckel***, Forschungszentrum Jülich, Germany **INVITED**

The discovery of the Giant Magnetoresistance GMR effect triggered the evolution of Spintronics, i.e. information storage, information processing and information transport using the spin of the electron. While the first Spintronic devices were merely transition metal multilayers, the interest has shifted to include transition metal oxide systems, laterally structured films and magnetic nanoparticles. Scattering techniques applied to model systems are ideal to provide fundamental microscopic information on the spin and domain structure.

In this contribution, we will give an overview highlighting the capabilities of modern neutron and synchrotron x-ray techniques. We will show that neutron scattering under grazing incidence is able to provide unique depth resolved information on magnetization, magnetic correlations and magnetization dynamics relevant for basic and applied research on nanostructured magnetic materials and how synchrotron x-ray scattering can provide complementary element specific information. Examples for current research on patterned metallic multilayers, thin transition metal oxide films and magnetic nanoparticles will be given.

8:40am **NT+AS+MI-WeM3 Magnetic Properties of FePtRh Films and Multilayers Studied by Neutron Scattering**, ***D. Lott***, *J. Fenske*, Helmholtz-Zentrum Geesthacht, Germany, *G.J. Mankey*, Univ. of Alabama, *W. Schmidt, K. Schmalzl*, Forschungszentrum Juelich, Germany, *E. Tartakowskaya*, National Academy of Science, Ukraine, *H. Amabye*, ORNL, *F. Klose, A. Mulders*, ANSTO, Menai, Australia, *A. Schreyer*, Helmholtz-Zentrum Geesthacht, Germany, *V. Lauter*, ORNL

Ordered FePt alloys with $L1_0$ structure are known as materials with FM order and a high magnetic moment of Fe providing a large magnetization. The large atomic number of Pt on the other hand results in a high magnetic anisotropy. If grown in thin films, the high anisotropy often results in perpendicular magnetization which is the preferred orientation for current magnetic recording media. One way to control the magnetic properties in these materials is through the introduction of a third element into the crystal matrix e.g. Rh. When Rh is added to replace Pt in the equiatomic alloy, new magnetic phases emerge. Here neutron diffraction studies on the magnetic properties of different thick $Fe_{50}Pt_{50-x}Rh_x$ films in dependence on temperature and external magnetic fields allowed us to investigate the rich phase diagram of the system for thin films, e.g. the transition from the FM to AF state in the system with increasing Rh concentration. In particular films with a Rh concentration of about 10% show a temperature dependent AF-FM transition. From the neutron data it was moreover possible to determine the magnetic configurations in dependence on concentration, temperature and magnetic field on a microscopic scale. Based on the observed results a theoretical model considering the changes in the anisotropies could be developed. In a next step magnetic multilayer consisting of $Fe_{50}Pt_{50-x}Rh_x$ bilayers with different Rh concentrations were grown and studied by polarized neutron reflectivity to investigate the magnetic interactions along the lattice matched interfaces. First results will be presented here.

9:00am **NT+AS+MI-WeM4 Spectroscopic and Magnetic Characterization of the Spin-Crossover Transition in Thin Films of $Fe(C_{12}H_8N_2)_2(NCS)_2$**, ***E.C. Ellingsworth***, *G.J. Szulczewski*, The University of Alabama, Tuscaloosa, *V. Lauter*, Oak Ridge National Laboratory

The octahedral complex bis(1,10-phenanthroline)dithiocyanate iron(II), $Fe(phen)_2(NCS)_2$, is known

to exhibit an abrupt transition between a high and low magnetic spin state from 170 – 180 K in the

bulk phase. As a result, $Fe(phen)_2(NCS)_2$ is an interesting organic semiconductor to study charge and

spin transport in thin films. We synthesized and characterized $Fe(phen)_2(NCS)_2$ according to literature

procedures. Thin films of $Fe(phen)_2(NCS)_2$ were made by vapor deposition onto a variety of substrates

including Si, KBr, Au and Al and characterized by infrared and photoelectron spectroscopy, SQUID

magnetometry, optical microscopy, and polarized neutron reflectometry. The films were found to be

very sensitive to water vapor under ambient conditions, which complicates the structural, chemical and

magnetic analysis of the films. However, appropriate capping layers can be deposited onto the

$Fe(phen)_2(NCS)_2$ thin films to protect them from water vapor before removal from the vacuum system. The

differences in the magnetic behavior of the thin films will be compared to the bulk phase.

***** Postdoc Award Finalist

9:20am **NT+AS+MI-WeM5 Nanoscopic Magnetic Phase Separation at the $SrTiO_3(001)/La_{1-x}Sr_xCoO_3$ Interface**, *M. Sharma, M.A. Torija,* Univ. of Minnesota, *J. Gazquez, M. Varela,* ORNL, *J. Schmitt, C. He,* Univ. of Minnesota, *J.A. Borchers, M. Laver,* NIST, *S. El-Khatib,* American University of Sharjah, *V. Lauter, H. Ambaye, R. Goyette,* ORNL, ***C. Leighton***, Univ. of Minnesota **INVITED**

The remarkable functionality of complex oxides, when combined with the favorable lattice matching that is possible at their interfaces, provides many opportunities for new physics and applications. The perovskite manganites and cobaltites are excellent examples, being of interest in gas sensing, catalysis, and as electrodes in ferroelectric memory and solid oxide fuel cells. From the magnetism perspective they have potential for high conduction electron spin polarization, and a variety of functional ground states. However, the same delicate balance between phases that provides such impressive functionality also leads to a serious problem; it can be difficult to maintain desired properties (e.g. high spin polarization and conductivity) close to the interface with a dissimilar oxide. This is exemplified by magnetic tunnel junctions for example, where the interface spin polarization is suppressed and drops rapidly with temperature. In this work, using SrTiO3(001)/La1-xSrxCoO3 [1] as a model system, we have combined epitaxial growth by high pressure oxygen sputtering with atomic-level stuctural characterization (including STEM/EELS imaging [2]), conventional magnetometry, electronic transport, small-angle neutron scattering, and polarized neutron reflectometry. We observe the usual degredation in magnetization and conductivity in the very thin film limit. We demonstrate that this is due to nanoscopic magnetoelectronic phase separation in the interface region [3]. Essentially, nanoscopic ferromagnetic (FM) clusters form in an insulating non-FM matrix near the interface, resulting in reduced magnetization and conductivity, even at compositions that display no such phase separation in bulk. STEM/EELS depth profiling of the chemical composition reveals that this effect has a chemical origin, being due to subtle depth-wise variations in Sr and O content, resulting in reduced hole doping near the interface. Simple thermodynamic and structural arguments for the origin of these variations are provided, based on Sr dissolution energies and the critical link between srain state and O vacancy concentration provided by O vacancy ordering [2,3].

Work at UMN supported by NSF and DoE (neutron scattering). Work at ORNL supported by DoE. Work at UCM supported by the European Research Council.

[1] Torija, Sharma, Fitzsimmons, Varela, Wu and Leighton, *J. Appl. Phys.* **104** 023901 (2008).

[2] Gazquez, Luo, Oxley, Prange, Torija, Sharma, Leighton, Pantiledes, Pennycook and Varela, Nano. Lett. **11** 973 (2011).

[3] Torija, Sharma, Gazquez, Varela, He, Schmitt, Borchers, Laver, El-Khatib, Maranville and Leighton, published online, Adv. Mater. (2011).

10:40am **NT+AS+MI-WeM9 Study of $L1_0$ Ordering in ^{57}Fe/Pt Multilayers**, ***K. Srikanti***, Ugc-Dae, Csr, India

Ordered $L1_0$ FePt, FePd and CoPt alloy thin films have large magnetic anisotropy constants suitable for high-density recording media. The $L1_0$ ordered phase is obtained with post growth annealing at high temperatures. However, the high temperature annealing leads to grain growth. The present work is an attempt to lower the transition temperature starting with multilayer precursors. The evolution of the structural and magnetic properties of Si(sub) [^{57}Fe(19Å

)/Pt (25Å)]$_{x10}$ multilayers as a function of vacuum annealing at different temperatures is studied. The film thickness is selected to have equi-atomic stoichiometry. The multilayers are prepared by ion beam sputtering. X-ray reflectivity (XRR), X-ray diffraction (XRD), and magneto optical Kerr effect (MOKE) and conversion electron Mössbauer spectroscopy (CEMS) are used to characterise the as-deposited and annealed multilayers. Using XRR it is observed that due to intermixing FePt alloy formation takes place with annealing. The XRD indicated the presence of superstructure peaks at 350^{0}C and above.Mössbauer measurements indicated a clear evidence for the strong exchange coupling between the soft fcc FePt and hard fct FePt phase. The results indicate that the multilayer structure does not transform directly to the ordered fct FePt, rather first an fcc FePt phase is formed and subsequently it gets converted in to the fct FePt phase as a function of annealing. A detailed study on stoichiometric FePt system embedded in Carbon matrix prepared by ion beam sputtering technique will also be discussed.

Few preliminary results of polarised neutron reflectivity measurements on FePt/FeNi exchange spring magnets will be discussed.

11:00am **NT+AS+MI-WeM10 Influence of Capping Layer Rigidity on Properties of Supporting Temperature Sensitive Hydrogel Polymers Using Neutron Reflectivity**, ***M. Dubey***, Los Alamos National Laboratory, *M.S. Jablin*, Carnegie Mellon University, *M. Zhernenkov*, Los Alamos National Laboratory, *R. Toomey*, University of South Florida, *J. Majewski*, Los Alamos National Laboratory

Temperature sensitive hydrogel polymers are utilized as responsive layers in various applications. While the polymer's native characteristics have been studied extensively, details concerning its properties during interaction with bio-related structures are lacking. This work investigates the interaction between a thermoresponsive polymer cushion and different lipid membrane capping layers probed by neutron reflectometry. N-isopropylacrylamide copolymerized with methacroylbenzophenone first supported a lipid bilayer composed of 1,2-Dipalmitoyl-*sn*-Glycero-3-Phosphoethanolamine (DPPE) and subsequently 1,2-Dipalmitoyl-*sn*-Glycero-3-Phosphocholine (DPPC). The polymer-membrane systems were investigated above and below the polymer lower critical solution temperature (37 and 25 °C). While the same cushion supported each lipid membrane, the polymer hydration profile and thickness were markedly different for DPPE and DPPC systems. Since DPPE and DPPC have different bending rigidities, these results establish that the polymer-membrane interaction is critically mediated by the mechanics of the membrane, providing better insight into cell-hydrogel interactions. There has been increased interest in the effect of matrix elasticity on cell lineage specification. Polymeric matrices with known stiffness are utilized as supports to understand the physical effects of *in vivo* tissue microenvironment for therapeutic uses of stem cells. This work focuses on the infleunce of a capping layer on the mechanical properties of the underlying support.

Actinides and Rare Earths Focus Topic
Room: 209 - Session AC+MI-WeA

Magnetic and Electron Correlation Effects in Actinides and Rare Earths

Moderator: J.G. Tobin, Lawrence Livermore National Laboratory

2:00pm **AC+MI-WeA1 Electronic Structure Theory of Complex Ordered Actinide Materials**, ***P.M. Oppeneer***, Uppsala University, Sweden **INVITED**

Actinide materials display many complex and correlated behaviors that originate from the special properties of the open f-shell atom embedded in a specific material's environment. First-principles investigations provide a route to assess these anomalous phenomena in a materials specific way, providing direct, fundamental insight.

Here we consider recently obtained *ab initio* modeling results for actinide materials that are in the focus of current interest: actinide oxides, such as NpO_2, PuO_2, and higher-oxides, U_3O_8, and Np_2O_5, the hidden order (HO) material URu_2Si_2, and correlated plutonium compounds.

NpO_2 is one of the very few materials in which complex multipolar order has been identified. Using the density-functional theory (DFT)-based LDA+*U* method we provide a first-principles theory of multipolar order and superexchange in NpO_2. DFT+*U* calculations offer a precise microscopic description of the 3***q***-antiferro ordered phase. We find that the usually neglected higher-order multipoles (electric hexadecapoles and magnetic triakontadipoles) are at least equally significant as the electric quadrupoles and magnetic octupoles [1].

We further investigate light actinide oxides in higher oxidation states, such as U_3O_8, PuO_{2+x}, and Np_2O_5, for which non-collinear magnetic ordering is predicted. The possible further oxidation of PuO_2 to PuO_{2+x} is studied using DFT+*U* calculations in combination with x-ray absorption measurements [2].

The Pu monochalcogenides are intriguing materials, in which a correlated temperature gap develops, reminiscent of the behavior seen in Kondo insulators. Using dynamical mean field theory (DMFT) in comparison to LDA+*U* calculations, we show that dynamical self-energy fluctuations are important for the formation of an unusual gap. Static approximations to the self-energy as the LDA+*U* fail to provide a gap.

For URu_2Si_2 we report extensive electronic structure investigations [3], using full-potential LSDA, LSDA+*U*, and DMFT approaches to assess the origin of the hidden order. Our investigation show that the itinerant f-electron picture provides an excellent description of the materials properties of this fascinating compound. The Fermi surface which is crucial for the HO transition and the occurrence of unconventional superconductivity is accurately given. Our study points to the formation of long-lived spin fluctuations that are the driving quasiparticles for the HO.

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3. P.M. Oppeneer, J. Rusz, S. Elgazzar, M.-T. Suzuki, T. Durakiewicz, and J.A. Mydosh, Phys. Rev. B **82**, 205103 (2010).

2:40pm **AC+MI-WeA3 Anomalous Quasiparticle Dynamics in the Hidden Order state of URu_2Si_2**, ***T. Durakiewicz***, *G.L. Dakovski, Y. Li, S.M. Gilbertson, G. Rodriguez, A.V. Balatsky, J.X. Zhu, K. Gofryk, E.D. Bauer, P.H. Tobash, A. Taylor, J.L. Sarrao,* Los Alamos National Lab, *P.M. Oppeneer,* Uppsala Univ., Sweden, *P.S. Riseborough,* Temple Univ., *J.A. Mydosh*, Leiden Univ., the Netherlands **INVITED**

An exotic phase of unknown nature emerges from a heavy fermion state in URu_2Si_2 at $T_0 = 17.5$ K. The nature of this hidden order (HO) state is being vigorously debated, while the massive removal of entropy due to the HO transition evades explanation. Here we use time-and angle-resolved photoemission spectroscopy (tr-ARPES) to elucidate the itinerant nature of HO. We show how the Fermi surface is renormalized by shifting states away from the Fermi level at specific hot spots. By measuring the ultrafast dynamics we identify the location and lifetime of the quasiparticle states forming at the hotspots. We find that the quasiparticle lifetime increases from 42 fs to few hundred fs across the HO transition, and the hidden order parameter is related to the anisotropic gapping of the Fermi surface.

4:00pm **AC+MI-WeA7 Advanced X-ray Spectroscopies on 4f and 5f Systems**, ***J. Bradley***, *M. Lipp,* Lawrence Livermore National Laboratory, *A. Sorini*, SLAC National Accelerator Laboratory

Photon-in photon-out x-ray spectroscopies allow for a bulk-sensitive, high-pressure compatible look at rare earth and actinide electronic structure. The techniques couple to well-defined and meaningful quantum mechanical observables, including orbital occupation number and magnetic moment. These observables are key differentiators between theoretical treatments of strongly correlated systems, and they also provide meaningful and correct intuitive understanding. Here we will present an selection of measurements, both at ambient and high pressure, that exemplify the kind of insight these techniques can provide. In particular, we will address the question of rare earth volume collapse, where considerable controversy has existed between competing (Mott vs. Kondo) theoretical treatments.

4:20pm **AC+MI-WeA8 Hard X-Ray Photoelectron Spectroscopy and Electronic Structure of Single Crystal UPd_3, UGe_2, and USb_2**, ***M.F. Beaux***, *T. Durakiewicz, J.J. Joyce, E.D. Bauer, J.L. Sarrao,* Los Alamos National Laboratory, *L. Moreschini, M. Grioni,* Ecole Polytechnique Federale, Switzerland, *F. Offi,* Universita Roma Tre, Italy, *M.T. Butterfield,* KLA-Tencor, *G. Monaco,* European Synchrotron Radiation Facility, France, *G. Panaccione,* Laboratorio Nazionale TASC-INFM-CNR, Italy, *E. Guziewicz*, Polish Academy of Sciences

Hard X-ray Photoelectron Spectroscopy (HAXPES) with 7.6 keV photons has been performed on single crystals of UPd_3, UGe_2, and USb_2 at the European Synchrotron Radiation Facility (ESRF). The greatly reduced surface sensitivity of HAXPES enabled observation of the bulk core levels in spite of surface oxidation. An 800 meV splitting within the Sb 3d core level was observed. The splitting of the Sb core levels is attributed to manifestations of two distinct Sb binding sites within the USb_2 single crystal as supported by consideration of interatomic distances and enthalpy-of-formation. Photoelectron mean-free-path vs oxide layer thickness considerations were used to model the effectiveness of HAXPES for probing bulk features of in-air cleaved samples.

4:40pm **AC+MI-WeA9 Actinide Dioxides under Pressure**, ***L. Petit***, Daresbury Laboratory, UK

The self-interaction corrected local spin density approximation is used to investigate the oxidation of actinide dioxides under pressure. The methodology enables us to determine the ground state valency configuration of the actinide 5f electrons and to study the localization/delocalization transition that occurs under pressure. We argue that this delocalization facilitates the oxidation of the actinide dioxides and present results for the estimated transition pressures.

5:00pm **AC+MI-WeA10 Hybridization and Electronic Structure in Pu Compounds**, ***J.J. Joyce***, *T. Durakiewicz, K.S. Graham, M.F. Beaux, E.D. Bauer, J.N. Mitchell, T.M. McCleskey, E. Bauer, Q.X. Jia, R.L. Martin, J.X. Zhu, J.M. Wills,* Los Alamos National Laboratory, *L. Roy,* Savannah River National Laboratory, *G.E. Scuseria*, Rice University

The electronic structure of Pu materials is directly tied to the details of the 5*f* electron bonding and hybridization. In compounds where direct 5*f*-5*f* bonding is negligible due to crystal structure and wavefunction overlap, hybridization is the key component for 5*f* electron influence on electronic properties. We examine two strongly correlated materials, PuCoGa5 and PuO2 that span the range of interesting materials from Mott insulator to heavy fermion superconductor. The synergy between synthesis, spectroscopy and modeling has provided a unique opportunity to explore details of the energy and crystal momentum dependence of Pu compound electronic structure through angle-resolved photoemission on single crystal samples and advanced modeling based on theories beyond density functional theory.

The strength of the 5*f* electron hybridization may be quantified through dispersion in 5*f* electron peaks from the angle-resolved photoemission. In the case of PuO2, we see over two eV of dispersion in the hybridized (O 2p - Pu 5*f*) valence band. For PuCoGa5, the quasiparticle peak at the Fermi energy shows 50 meV or more of dispersion in reciprocal space over a range covering slightly less than half the zone center to zone boundary. We are unable to follow the peak dispersion beyond this point as it crosses above the Fermi energy. These energy dispersions place significant constraints on models, which might be used to describe the electronic structure of these strongly correlated materials. For PuCoGa5, models, which place the 5*f* electrons in a localized configuration without significant hybridization, would not agree with the experimental results. In the case of PuO2, the dispersion measured in photoemission agrees well with the

hybrid functional calculations for PuO2 and further support the increase in hybridization moving from ionic UO2 to covalent PuO2.

5:20pm **AC+MI-WeA11 Structure and Magnetic Properties of Actinide-Based Thin Films**, ***L. Havela***, Charles University, Czech Republic, *N.-T. Kim-Ngan*, Pedagogical University Cracow, Poland, *A. Adamska*, Charles University, Czech Republic, *A.G. Balogh*, TU Darmstadt, Germany, *T. Gouder*, European Commission, JRC Institute for Transuranium Elements, Germany **INVITED**

Actinide-based sputter deposited films were so far used in the context of surface-science studies (such as [1]) and for exploration of electronic structure by photoelectron spectroscopy (e.g. [2,3]). In addition, sputter deposition was used in attempts to synthesize amorphous uranium alloys for ex-situ studies of magnetic properties. Such early (late 1980's) attempts in U.S. [4] or Japan [5] were undertaken in simple setups and lack proper diagnostics of the deposited material. Considering strong electropositivity of U, oxidation has to be suspected for films prepared in HV conditions. More recently, U metal in multilayers with possibility of epitaxial growth were sputter deposited with the aim to induce uranium magnetic moments [6]. We have used sputter deposition to investigate structure and magnetic properties of various U-based compounds as a function of deposition conditions (deposition rate, substrate type and temperature). Employing diagnostics by XPS, Glancing Angle XRD, and RBS, it was established that UN films have a long-term stability, which allows comfortably to make ex-situ studies over months. The reason can be seen in pronounced compressive residual strains, imposed during the deposition, which prevent progressing the surface oxidation into the bulk of several hundred nm thick films. Departing more from a fully crystalline state, the antiferromagnetism of UN is masked by a weak ferromagnetism, as usual for nanograined AF structures, and finally both moments and their order disappears [7]. Similar suppression of magnetism was found for ferromagnetic US [8].

Recently we undertook sputter-deposition experiments on Fe-rich U-Fe alloys derived from the Laves phase UFe_2, which combines the 3*d* and 5*f* magnetism in a compound with a relatively high Curie temperature (T_C = 162 K). An Fe-excess is expected to increase the T_C value markedly. Nanocrystalline material obtained up to the stoichiometry $UFe_{2.3}$ by splat cooling, with the excessive Fe atoms entering the U sublattice has T_C enhanced up to 230-240 K. More Fe leads to the segregation of α-Fe. We succeeded to synthesize amorphous films by U and Fe co-sputtering, with stoichiometry up to UFe_3. T_C is enhanced up to 450 K in this case.

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[5] S. Itoh et al., Physica B 281-282 (2000) 230.

[6] R. Springell et al., Phys. Rev. B 77 (2008) 064423.

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Magnetic Interfaces and Nanostructures Division
Room: 105 - Session MI-WeA

Spintronics, Magnetoelectronics, Multiferroics, and Dilute Magnetic Semiconductor Applications
Moderator: E. Vescovo, Brookhaven National Laboratory

2:00pm **MI-WeA1 Novel Properties of Topological Insulator Thin Films Prepared by Molecular Beam Epitaxy**, ***Q.-K. Xue***, Tsinghua University, China **INVITED**

We have grown topological insulator thin films of Bi_2Te_3, Bi_2Se_3 and their alloys on Si(111), 6H-SiC(0001) and sapphire substrates by using state-of-art molecular beam epitaxy (MBE). We studied nontrivial surface states and their thickness-dependence of the films by *in situ* angle resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy/spectroscopy (STM/STS). By direct imaging standing waves associated with magnetic and nonmagnetic impurities and steps on Bi_2Te_3 and Bi_2Se_3 (111) surfaces, we show that the topological states have a surface nature and are protected by the time reversal symmetry. We demonstrated the high mobility of the Bi_2Se_3 films by direct observation of Landau quantization. We also studied the growth of superconducting and magnetic thin films on the topological insulator films. Implication on probing Majorana fermions and topological magneto-electric effect will be discussed.

2:40pm **MI-WeA3 Kondo Effect in a Molecular Machine**, ***U.G.E. Perera****, *Y. Zang*, *H. Kersell*, Ohio Univerisity, *G. Vives*, *G. Rapenne*, CNRS, Cemes, France, *S.-W. Hla*, Ohio University

Due to the continuous miniaturization of existing devices, artificial molecular machines have emerged as a new field in nano-science with the aim of developing novel motion systems on a single-molecule level. Here, we report the spin-electron interactions and local vibration signature of an artificially synthesized double-decker molecular rotor 4Fc3SEt on Au(111) surface for the first time using a low temperature scanning tunneling microscopy and spectroscopy at 5 K. The 4Fc3SEt molecule has an upper-deck capability of rotating around the sandwiched metal ion as its rotational axis. The upper-deck has five arms and four of these have ferrocene units attached to pi-ring. A spin-active iron atom is caged at the center of each ferrocene unit. The lower-deck of the molecule is the stator and includes three SEt groups which are designed to anchor on to the Au(111) substrate. At 80 Ktemperature, most of the molecular rotors were found to be rotating due to thermal excitation. However, when the sample was cooled down to 5 K temperature, stationary conformation of the molecular rotors was determined by high resolution STM images. We probe the spin-electron interactions between the spin of the iron atom inside the molecule, and the surface state free electrons of Au(111) by monitoring the differential conductance (dI/dV) tunneling spectroscopy. Furthermore, by measuring dI2/dV2-V spectroscopy on the ferrocene units, the vibration signature of M(Cp)2 was identified. Both signatures reveal a site dependent orbital effect in the upper rotator arm. This work opens a novel avenue of molecular machines future nanoscale spintronic and mechanical applications. This work is supported by the US Department of Energy Basic Energy Sciences grant no. DE-FG02-02ER46012 and NSF OSIE 0730257.

3:00pm **MI-WeA4 Spin-Polarized Photoemission of Long-Range Metal-Organic Supramolecular Networks**, ***S.Z. Janjua***, University of Missouri - Kansas City, *E. Vescovo*, Brookhaven National Laboratory, *K.I. Pokhodnya*, North Dakota State University, *A.N. Caruso*, University of Missouri - Kansas City

Preliminary spin-resolved photoemission studies of in-situ deposited supramolecular networks were completed at the National Synchrotron Light Source, beamline U5UA. The molecular networks were grown on metallic surfaces with and without a remanent magnetic moment with the intention of studying the influence of the interfacial dipole on the induced moment of the molecules and their long-range order.

4:00pm **MI-WeA7 Spin Transport Phenomena in Nanostructures with Non-Collinear Magnetic Moments**, ***M. Chshiev***, SPINTEC, UMR 8191 CEA/CNRS/UJF Grenoble, France **INVITED**

Spintronic phenomena in magnetic nanostructures with non-collinear spin configurations have been of major interest for scientists and engineers. Among the most important phenomena arising from non-collinearity of magnetic moments and which has tremendous impact on spintronics [1] is current induced magnetization switching caused by spin transfer torque [2] (STT). The latter continues to generate interest for spin electronic applications such as magnetic random access and domain wall racetrack memories, spin torque oscillators and detectors. Among the most favorable candidates for realization of STT devices are crystalline magnetic tunnel junctions (MTJ) where Bloch state symmetry based spin filtering may lead to extremely high TMR ratios [3] (MTJ).

The first part of this talk will include theory of non-equilibrium spin currents and the corresponding spin transfer torques in MTJs with non-collinear moments. Calculations are based on the Keldysh formalism in which the non-equilibrium Green functions are calculated within a tight-binding model and free electron models. The properties of spin transfer torque and spin currents as a function of applied bias, barrier thickness and distance from the interface in the free layer will be discussed [4].

The second part of the presentation will be devoted to phenomenon of interlayer exchange coupling which also results from equilibrium spin currents in non-collinear magnetic configurations. In particular, using ab-initio and tight-binding approaches, we will address the impact of interfacial oxidation conditions on amplitude of IEC in MTJs [5] as well as the importance of occupation numbers on period of IEC oscillation as a function of ferromagnetic electrode thickness [6] and dynamics of exchange coupled magnetic moments.

In conclusion, theory of voltage induced switching in magnetically frustrated bulk materials will be presented [7].

***** Postdoc Award Finalist

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4:40pm **MI-WeA9 Concepts based on Magnetoelectrics and Half-Metals for Spintronic Applications**, ***K.D. Belashchenko***, University of Nebraska-Lincoln **INVITED**

I will discuss two new concepts of interest for voltage-controlled magnetism and for efficient high-current spin injection in semiconductors, as well as our computational studies of magnetic materials that may be employed in such devices.

First, I will explain the concept of a boundary magnetization carried by a magnetoelectric antiferromagnet, which can be used to induce a switchable equilibrium exchange bias in a proximate ferromagnet. This effect, demonstrated experimentally using magnetoelectric Cr_2O_3, can be utilized in non-volatile magnetoelectric memory and spin field-effect transistors. However, for these purposes the Cr_2O_3 Néel temperature of 307 K is too low. Using first-principles calculations, we predict that it can be increased by introducing boron as a substitutional dopant in the anion sublattice, whereas transition-metal dopants are detrimental. Compressive in-plane strain was also found to be favorable.

Next, I will discuss the possibility of Ohmic spin injection in semiconductors without using Schottky or tunnel barriers. Usually such a high-resistance interfacial barrier is used to overcome the conductivity mismatch problem, but this barrier limits the injected current density. A half-metal used as a spin injector overcomes this problem at zero temperature, but the situation at finite temperatures is nontrivial. I will argue that the two-current model is inapplicable to half-metals, and that barrier-free spin injection from a half-metal may be possible even at finite temperatures. I will present an intuitive model summing up multiple scatterings at the interface, as well as direct calculations of the spin injection efficiency in a simple tight-binding model with averaging over thermal spin fluctuations.

There is much interest in Gd-doped EuO as a half-metal that could be used as a spin injector. Gd doping (and, more controversially, O deficiency) sharply enhances the Curie temperature from 69 K up to as much as 170 K. I will report the results of first-principles studies of exchange interaction in Gd-doped EuO. In the virtual crystal approximation the indirect exchange through the conduction band qualitatively explains the observed doping dependence of the Curie temperature. We also considered EuO supercells with one or more substitutional Gd atom, as well as with an oxygen vacancy, and found deviations from the virtual-crystal behavior that can be associated with local lattice relaxations.

Time permitting, I will also show how first-principles calculations for large supercells with noncollinear spins can be used to analyze the spin-disorder contribution to the electric resistivity of magnetic metals.

5:20pm **MI-WeA11 Magnetic, Structural and Morphological Characterization of Self Assembled Dilute Magnetic Mn_xGe_{1-x} Quantum Dots**, ***J.K. Kassim***, *J.A. Floro, P. Reinke, C.A. Nolph*, University of Virginia

Group IV dilute magnetic semiconductors (DMS) are candidates for the development of spin based devices due to their compatibility with the traditional semiconductor technology. We have grown heteroepitaxial Ge1-xMnx quantum dots (QDs) on Si (001) by molecular beam epitaxial co-deposition, with x ranging from 0.02 – 0.22. There is evidence in the literature for room-temperature ferromagnetism in Mn-doped Ge quantum dots. Using atomic force microscopy, in situ scanning tunneling microscopy, transmission electron microscopy, and in situ scanning Auger mapping, our goal is to clearly ascertain how and where Mn incorporates in our films, especially where the magnetically-active Mn resides, and in so doing to contribute to our understanding of the basic origin of ferromagnetic (FM) ordering in this system. Morphology of the QD's up to 5 at.% nominal Mn atomic fraction mirror those observed in pure Ge QDs grown at identical temperatures and deposition rates. The standard "hut cluster" islands bound by {105} facets are observed followed by the introduction of dome clusters at larger Ge thicknesses. Noticeable changes in morphology, QD's density and mean volume become apparent for the highest Mn contents. Further increase in Mn content promotes introduction of rods believed to be a germanide phase. Field cooled hysteresis loops obtained by vibrating sample magnetometry with an in-plane external magnetic field demonstrate ferromagnetic behavior at 5K, with a maximum magnetization saturation of 2.1μB per Mn ion and a coercivity of 250 Oe recorded for x=0.02. Ferromagnetism disappears above 70K, and is not improved by increasing average Mn content of the films. The saturation moment on a per atom basis is seen to decrease with an increase in Mn content. While we cannot yet isolate any specific island type, or the wetting layer, as being primarily responsible for the ferromagnetism, we have shown that dome clusters are not a prerequisite to ferromagntism. This work is supported by the National Science Foundation under grant number DMR-0907234.

5:40pm **MI-WeA12 Alterations in the Electronic Band Structure and Magnetic Properties of EuO Films via Rare Earth Doping**, ***J.A. Colón Santana****, *J. An, N. Wu, K.D. Belashchenko,* University of Nebraska-Lincoln, *X. Wang, P. Liu, J. Tang,* University of Wyoming, *Ya. Losovyj,* Center for Advanced Microstructure & Devices, *I.N. Yakovkin,* National Academy of Science of Ukraine, *P.A. Dowben*, University of Nebraska-Lincoln

High quality films of EuO, $Eu_{0.096}Ce_{0.04}O$ and $Eu_{0.096}Gd_{0.04}O$ were successfully grown on a p-type Si (100) substrate via pulsed laser deposition (PLD). X-ray diffraction (XRD) results show that the addition of Gd changes the growth texture orientation from [001] to [111] with both films crystallizing in the expected rock-salt structure. Angular-resolved photoemission spectroscopy (ARPES) measurements confirms that the doping with Gd atoms have a strong influence in the electronic band structure of these films as well, revealing the presence of electron pockets around some of the high symmetry point in $Eu_{0.096}Gd_{0.04}O$ and $Eu_{0.096}Ce_{0.04}O$ films. There is confirmation of the indirect nature of the EuO electronic band gap suggesting a near semi-metallic character for the $Eu_{0.096}Gd_{0.04}O$ surface. Combined photoemission and inverse photoemission measurements suggests that under some circumstances the surface appears p-type apparent rather than the expected n-type and this unexpected result is likely due to a reconstruction of the highly polar (111) surface. The combination of Gd doping and oxygen vacancies does lead to an appreciable density of states at the Fermi level and is seen to affect the magnetic properties of these films.

***** Falicov Student Award Finalist

Magnetic Interfaces and Nanostructures Division
Room: 105 - Session MI-ThM

Emerging Magnetic Characterization and Results

Moderator: A.N. Caruso, University of Missouri-Kansas City

8:00am **MI-ThM1 The X-ray View of Ultrafast Nano Magnetism**, ***H.A. Durr***, SLAC National Accelerator Laboratory **INVITED**

Polarized soft x-rays have been used over the past 20 years to obtain fascinating new insights into nanoscale magnetism. The separation of spin and orbital magnetic moments, for instance, enabled detailed insights into the interplay of exchange and spin-orbit interactions at the atomic level. X-ray and photoelectron imaging techniques have revolutionized our understanding of magnetism of the ULTRA SMALL. In addition the now available polarized soft x-ray pulses with only few ps down to 100 fs duration allow us to observe the magnetic interactions at work in real time, i.e. they open the door to study ULTRA FAST magnetism. The ultimate goal of such studies is to understand how spins may be manipulated by ultrashort magnetic field, spin polarized current or light pulses. In this talk I will give an overview of achievements and the current status of probing magnetism of the ultra small and ultra fast using x-rays from synchrotrons [1-3] and more recently from x-ray free electron lasers.

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8:40am **MI-ThM3 Spectroscopy of Magnetic Thin Films**, ***S.N. Gilbert, N.H. Tolk***, Vanderbilt University

Recent studies of magnetic thin films and spintronic devices will be presented. Time-resolved Kerr Effect measurements of ferromagnetic/antiferromagnetic interfaces as a function of film layer thickness and antiferromagnetic spin orientation will be discussed. Magnetic and time-resolved spin characterization of novel spintronic devices and materials will also be shown.

9:00am **MI-ThM4 Detection and Control of Electronic Phase Competition in Complex Oxides**, ***T.Z. Ward***, Oak Ridge National Laboratory **INVITED**

Electronic phase separation is present in many complex material systems and has been linked to colossal magnetoresistance, high T_c superconductivity, and multiferroicity. Here, nanometer to micron sized regions of vastly different electronic and magnetic properties can coexist and compete within single crystal materials. We will discuss recent work on fabricating single crystal wires of electronically phase separated manganites to a size comparable to the domains of the electronic phases residing in the material; thereby allowing finite emergent regions to dominate device characteristics. This has given us a means to probe, observe and exploit properties which are *hidden* in unconfined systems. Transport measurements on simple confined structures reveal new properties such as ultrasharp jumps in resistivity, a reemergent metal-insulator transition, and discreet resistive hopping that are unseen in larger samples. We have found that these properties are also tunable through doping, strain, electric field and magnitude of confinement. This ability to control key elements of the underlying complex electronic correlations and observe the resulting changes in a material's behavior help answer questions about the fundamental physics that rule emergent phenomena in complex materials while opening the door to new device functionality.

9:40am **MI-ThM6 Room-Temperature Spin-Polarized Scanning Tunneling Microscopy of Topological Antiferromagnetic Nanopyramids on Mn_3N_2(001) Surfaces**, ***K. Wang****, *A.V. Chinchore, W. Lin, A.R. Smith*, Ohio University

Antiferromagnets play a critical role in spintronic applications such as pinning layers in magnetic memories. The development of spin-polarized scanning tunneling microscopy and spectroscopy (SP-STM/STS) has shown its unprecedented power in resolving the local spin and domain structures of antiferromagnetic surfaces down to atomic level.[1-6] While most efforts have been made on imaging metal surfaces at cryogenic temperatures, only a few have been devoted to the study of room-temperature magnetic systems.[4-6] Here we apply SP-STM/STS to study the local spin and magnetic properties of a technologically driven material system which exhibits layer-wise antiferromagnetism with a very high Néel temperature (>900 K)[7]. Mn_3N_2(001) thin films have been grown on MgO(001) substrates using ultra high vacuum plasma-assisted molecular beam epitaxy and transferred *in situ* to a home-built room-temperature SP-STM[8] for magnetic imaging. Results have shown that the surface exhibits a *topological spin pyramid* structure with alternating single Mn- and double MnN- layers, where the magnetism is strongly correlated with the surface topography. Using SP-STM with *dI/dV* mapping, different layers can be clearly distinguished due to their different conductance. These differences in the conductance are a result of not only the different chemical environments, but also the spin ordering and the broken symmetry at the surface. We will show that it is possible to separate the contributions from both the electronic and the magnetic structure by applying a small magnetic field. The field rotates the tip magnetization axis causing concomitant change in the magnetic sensitivity while keeping the electronic structure unchanged. The demonstrated ability of direct imaging at room-temperature of the surface antiferromagnetic terraces allows further (ongoing) studies on the interplay between structural defects such as anti-phase domain boundaries and the formation of intriguing antiferromagnetic domains. We gratefully acknowledge support from the Department of Energy and the National Science Foundation.

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10:40am **MI-ThM9 Growth Strategies for Mn Doping of Ge Quantum Dots: An STM Study of Reactions, Bonding and Phase Formation**, ***C.A. Nolph§, K.R. Simov, P. Reinke***, University of Virginia

Manganese doped, magnetic germanium quantum dots are predicted to be important building blocks for the future of spintronic devices. The combination of quantum confinement and carrier mediated ferromagnetism make these structures particularly interesting. The goal of this work is to understand and control the Mn environment within the Si(100), Ge wetting layer and Ge quantum dot (QD) systems and understand how it influences the magnetic properties. Samples were investigated primarily using scanning tunneling microscopy followed by magnetic analysis using a vibrating sample magnetometer and one sample with x-ray magnetic circular dichroism. An important materials question is the competition to form secondary phases in this system at elevated temperatures, particularly Mn5Ge3 and Mn11Ge8 which are both ferromagnetic (TC = 294 – 296 K). We investigate three routes for Mn doping of Ge QDs : (1) The investigation of the stability and evolution of Mn nanostructures on a Si(100)-(2x1) reconstructed surface as a function of annealing temperature up to temperatures typical for Ge QD growth. At an annealing temperature of approximately 316°C, Mn adatoms move into Si sub-surface sites and we observe an electronic effect consistent with acceptor dopants. (2) The use of a surface driven approach where Mn is deposited on the Ge QD surface and forms well-defined islands on the QD and wetting layer surface. We observed the behavior of the Mn islands during STM measurement with increasing annealing temperatures and how the islands evolved via ripening and migration across the surfaces. In addition the structure and bonding of the Mn islands specifically on the Ge {105} facets will be discussed. (3) The co-deposition of Ge and Mn throughout the Ge QD growth process. For route (3) the highest Mn concentration is 23% which results in only minor

***** Falicov Student Award Finalist

perturbations in the Ge QD growth (fewer and smaller Ge QDs), albeit secondary phases form on the surface. Lower concentration samples (5% and 8% Mn) yielded high quality quantum dots and no observable secondary phases on the surface. We presume that when secondary phases form, the majority of the Mn deposited is consumed to form the secondary phases. The competition to form secondary phases is investigated further utilizing scanning auger microscopy to map Mn and low energy electron microscopy to study the growth sequence as a function of Mn concentration. Magnetism results from one particular sample (Mn0.05Ge0.95 QD) indicate a ferromagnetic material with a Curie temperature above room temperature. We'd like to acknowledge our funding support from NSF CHE-0828318 and DMR-0907234.

11:00am **MI-ThM10 Novel Iron-Induced Structures on Gallium Nitride (0001) and (000-1) Studied Using Scanning Tunneling Microscopy and First Principles Theory**, ***W. Lin***, Ohio University Nanoscale and Quantum Phenomena Institute, *H.A.H. Al-Brithen*, Ohio University Nanoscale and Quantum Phenomena Institute and KAIN, King Saud Univ., Saudi Arabia, *K.K. Wang, A.V. Chinchore, M. Shi, Y. Liu, N. Takeuchi, A.R. Smith*, Ohio University Nanoscale and Quantum Phenomena Institute

There is much interest in the field of spintronics in which magnetic phenomena are combined with electronic properties to form a new class of materials with added device functionality. An essential area is that of magnetic nanostructures on the surface of semiconductors. Gallium nitride represents one of the most important next generation semiconductors. The possibility for long spin lifetimes in GaN make it attractive as a spintronic material as well.[1] From this perspective, it is important to explore the epitaxial growth of ferromagnetic layers such as Fe at the surface of GaN. New results for the growth of Fe-induced structures on wurtzite GaN will be presented in this talk.

These investigations are carried out using a custom-designed, home-built molecular beam epitaxy/scanning tunneling microscopy (MBE/STM) facility. Growth of iron on GaN is carried out using an Fe effusion cell and at a substrate temperature which is carefully selected in order to produce the highest quality atomically-smooth Fe-induced structures. It is found that the Fe-induced structures on Ga-polar GaN(0001) strongly depends on the presence of the pseudo-1×1 surface structure as a starting surface, and that under the correct conditions a clear 6×6 reconstructed island structure grows outward from the GaN step edges, as revealed in scanning tunneling microscopy images. First-principles theoretical calculations have been carried out which suggest a low-energy model for the 6×6 structure consisting of Fe atoms embedded within the pseudo-1×1 layer and with Ga adatoms at the top.

The results for N-polar GaN(000$\underline{1}$) are quite different. In this case, deposition of Fe onto a Ga-rich surface results in the formation of uniform-height Fe-induced islands having a 4×2 zigzag row structure. The zigzag rows orient along the high symmetry [11$\underline{2}$0] directions of the surface.

Efforts are also underway to investigate the chemical stoichiometry, and electronic and magnetic properties of these Fe-induced structures and to explore the evolution of these monolayer films as additional Fe and/or Ga is added to the surface.

This work has been supported by the U.S. Department of Energy, Office of Basic Energy Sciences (Grant No. DE-FG02-06ER46317). Additional support from the National Science Foundation (Grant No. 0730257) is also acknowledged.

Y.L. is now at Los Alamos National Laboratory, Los Alamos, NM.

N.T. was a visiting Presidential Scholar from the Universidad Nacional Autónoma de México during 2010-11.

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11:20am **MI-ThM11 Scanning Tunneling Microscopy and Spectroscopy Performed on Single Mn Monolayer on Wurtzite (000-1) GaN**, ***A.V. Chinchore***, *K.K. Wang, A.R. Smith,* Ohio University, *V. Ferrari, A. Barral*, University of Buenos Aires, Argentina

The III-V diluted magnetic semiconductors (DMS) are a new class of materials with promising applications in spintronics.[1] The low solubility of transition metal atoms into III-V semiconductor host has been a key concern in the successful development of DMS. This low solubility however was used to advantage by Lu et.al. to develop an ideal magnetic/semiconductor bi-layer [2]. Wang et.al. recently reported high density 2D Mn-Ga stripe phases on Ga-Polar GaN(0001) surface, with interesting atomic spin arrangement. [3] The N-Polar GaN(000$\underline{1}$) 1×1 structure offers an added advantage over the Ga-Polar structure, as the Mn atoms deposited on this surface are in closer proximity to the N atoms favoring the GaMnN bonding.

We have conducted a series of experiments aimed at understanding the behavior, electronic and magnetic properties of Mn atoms on N-Polar GaN(000$\underline{1}$) 1×1 surface. The experiments were conducted in a custom built MBE-STM system with *in-situ* sample transfer ability. The growth is monitored with reflection high energy electron diffraction (RHEED). The standard GaN(000$\underline{1}$) 1×1surface was prepared and was exposed to sub monolayer doses of Mn at various temperatures. It was observed that the behavior of Mn atoms on GaN(000$\underline{1}$) 1×1surface is highly sensitive to the substrate temperature (T_s). The low temperature Mn deposition, $T_s \sim 100$ °C, led to the formation of a metastable 3×3 structure which transformed to a more stable $\sqrt{3} \times \sqrt{3}$ R30° structure, when the sample is heated to $T_s \sim 120$ °C, as confirmed by RHEED. It was observed that the $\sqrt{3} \times \sqrt{3}$ R30° structure is stable up to 750 °C. The temperature dependent behavior of the structures suggests that the Mn atoms are *physisorbed* while forming the metastable structure and they are *chemisorbed* in the case of the stable $\sqrt{3} \times \sqrt{3}$ R30° structure. The STM measurements performed on the Mn 3×3 structure showing the metastable nature of the structure are presented as well are the STM and STS results showing the characteristics of $\sqrt{3} \times \sqrt{3}$ R30° surface. RHEED simulations confirming the surface atomic arrangement for the structure are presented. The theoretical calculations are performed using the first principles and the Tersoff-Hamann simulation method. The results indicate that the Mn atoms push the Ga atoms laterally in the surface ad-layer forming bonds directly with the bilayer N atoms. The funding from NSF and DOE for the project is greatly acknowledged.

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11:40am **MI-ThM12 Designing of Engineered Multiferroic Composites by Radical Enhanced Atomic Layer Deposition**, ***J.H. Choi***, *T.E. Quickel, S. Tolbert, J.P. Chang*, University of California Los Angeles

Multiferroic materials induced polarization under external magnetic field H, or induced magnetization under external electric field E. Magnetoelectric (ME) phenomena in multiferroic materials holds considerable promises because of their potential applications in spintronics, such as magneto-electric sensors, magneto-capacitive devices, and electrically driven magnetic data storage. The ultimate goal for practical device application of multiferroic materials is dependent on how to create strong ME coupling between different types of ferroic order. The strictive interaction between the piezoelectricity of the ferroelectric (FE) phase and the magnetostriction of the ferromagnetic (FM) phase lead to produce larger ME coefficients than single phase multiferroic materials. Thus, the research has been directed towards designing engineered multiferroic composite materials in the form of horizontal multilayer (2-2), vertical superstructures (3-1) or other nanoparticle composite structures (3-0) in a precise controlled manner.

In this work, the $BiFeO_3$ (BFO) and $Pb(ZrTi)O_3$ (PZT) thin film were synthesized by radical enhanced atomic layer deposition (RE-ALD). RE-ALD is a gas-phase technique in which precursor vapors are pulsed alternately into the reaction chamber and the thin film growth proceeds through surface reactions in a self limiting manner. The advantages of ALD include excellent conformality, simple and accurate thickness control and good uniformity on large areas. In order to demonstrate conformal deposition of engineered multiferroic materials in the form of 3-0 or 2-2 configuration, PZT and BFO was deposited onto a mesoporous $CoFe_2O_4$ (CFO) substrate by RE-ALD.

The mesoporous CFO films were found to be fully filled by ALD PZT and BFO. The composition and crystal structure of the PZT-CFO and BFO-CFO systems were confirmed by X-ray Photon Spectroscopy and X-ray Diffraction (XRD), respectively. More detail crystal structure were investigated by synchrotron XRD and extended x-ray absorption fine structure spectroscopy (EXAFS). The magnetic and ferroelectric properties for the PZT-CFO or BFO-CFO systems were characterized by a superconducting quantum interference device (SQUID) magnetometer and piezoresponse force microscopy (PFM). Magnetic properties such as coercive magnetic field (H_c) and saturation moment (M_s) were systematically analyzed on composite systems and the pure CFO substrate. In addition, The P-E loops for PZT-CFO and BFO-CFO thin films were measured at room temperature and the saturation polarization (P_s) and coercive field (E_c) were investigated with respect to thickness and crystal plan.

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

Magnetic Interfaces and Nanostructures Poster Session

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

Magnetic overlayers and bilayers of Ni and Co on Cu(001) have been investigated as a function of coverage, using X-ray Magnetic Circular Dichroism in X-ray Absorption Spectroscopy (XMCD-XAS) and Photoelectron Spectroscopy (PES). These studies were pursued at Beamline 4 at the Advanced Photon Source (APS).

Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344. This work is funded by the DOE Office of Science, Office of Basic Energy Science, Division of Materials Sciences and Engineering. The Advanced Photon Source (APS) is supported by the Director, Office of Science, Office of Basic Energy Sciences.

MI-ThP2 Microstructure, Static and Dynamic Magnetic Properties of Thin Co Films Obtained using DC-Magnetron Sputtering, ***S.A. Maklakov***, *I.A. Ryzhikov, K.N. Rozanov, A.V. Osipov, O.Yu. Kasurkin*, Institute for Theoretical and Applied Electromagnetics RAS (ITAE RAS), Russian Federation, *V.A. Amelichev*, Moscow State University, Russian Federation

Thin Co films possess high value of saturation magnetization, low coercivity and uniaxial magnetic anisotropy. These properties are necessary for high density storage devices, magnetic field sensors and applications for UHF electromagnetic radiation. Consequently Co is perspective material for such employments. There are many influences to affect magnetic film growth. The latter allows one to govern their properties in wide range. Comparative studies of microstructure and magnetic properties (static and dynamic) are essential to develop new approaches for directional obtaining of materials with given frequency dispersion of magnetic permeability.

The results of a comparative study of microstructure (TEM, GIXD), static (VSM) and dynamic (in the range of 0.01 to 10 GHz) magnetic properties of thin Co films are presented. The objects studied were rectangular films (60 x 600 mm) of 20 nm thick on poly(ethylene terephthalate) substrate. High purity (99,95%) cobalt disk target and a rotating drum as a substrate holder was used to obtain Co films.

Under a certain sputtering conditions two different types (with ferromagnetic resonance at 2 and 6 GHz) of Co films were obtained. Both types of films are of nanocrystalline structure. The increase of crystalline size (from 7 to 90 nm) along with the increase of coercivity (from 17 to 110 Oe) and the increase of resonant frequency (from 2 to 6 GHz) was discovered.

Uniaxial crystalline texture discovered was found to effect resonant frequency. When the texture axis is in the film plane, mechanical bending of Co film may cause resonance frequency varying up to 1 GHz. Perhaps the effect is due to magnetostriction mechanism [1].

The relationship obtained allows one to develop new pathways for magnetic materials production.

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MI-ThP3 A Facile and Controllable Two-Step Electrodeposition Technique in Synthesis of Nanostructures of Metal Oxides on Carbon Nanotube S, ***J. Yang***, *S. Gunasekaran*, University of Wisconsin-Madison

The nano dimensions of materials are comparable to the size of the target analyte biomolecule, higher catalytic reaction, better affinity binding or more efficient molecule-capturing may occur, leading to high sensitivity. And it is possible to use nanoparticle tags for designing electrical bioaffinity assays with remarkable sensitivity and multiplexing ability. So far, efforts have always been made to design novel nanomaterials useful in solving emerging bioanalytical problems such as rapidness, anti-interfering ability, specificity, stability and sensitivity. Synergies of nanocomposite materials, generally retaining the functional properties of each component and possibly yield synergistic effects via cooperative interactions, have exploited a new area to miniaturize and optimize nano-scale sensors and electronics. The synergistic interesting new features include but not limited to increased surface area, enhanced electrocatalytic activities, improved biocompatibility, promoted electron transfer and better invulnerability against intermediate species. A lot of efforts have been made to fabricate nanocomposite materials of metals/metal oxides nanostructures and carbon materials, using a number of techniques, including sputtering, sol–gel, hydrothermal, microwave and electrodeposition from different precursor solutions containing complex agents. Among these, electrodeposition is the easiest, most controllable, environment-friendly and robust technique for synthesis of metal/ metal oxides NPs, in which, the size, density, composition and even the shape of NPs could be well-controlled by electrodeposition potential, time, concentration and composition of metal precursor solutions.

Herein, we report a general two-step approach of electrodeposition useful in facile, controllable and 'green' electrochemical synthesis of metal oxide NPs onto carbon supports, using carbon nanotubes (CNTs) as an example. First, metal nanostructures were electrochemically deposited onto carbon supports at a constant potential with the density, size, shape and elctrocatalytic activities of the produced nanostructures well-controlled by the time and deposition potential applied as well as the concentration of the precursor solution. Then the as-deposited metallic nanostructures were oxidized into metal oxide nanostructures by repetitive potential cycling with extent of oxidation and generation of metal oxides controlled by the number of potential circles.The as-synthesized metal oxides-CNTs composites were characterized and applied as a glucose sensor for illustration of their electrocatalytic properties.

MI-ThP4 Magnetic Properties and Size Control of $Zn_{0.95}Mn_{0.05}O$ Nanorods Deposited by Pulsed Laser Deposition, ***T.C. Wu***, *Y.C. Yeh, D.R. Liu, D.Y. Chiang*, National Applied Research Laboratories, Taiwan, Republic of China

The well-aligned ZnO nanorods with 5 at.% of Mn doping ($Zn_{0.95}Mn_{0.05}O$) were deposited on silicon (100) substrates by pulsed laser deposition at three different substrate temperatures ranged from 600 ℃ to 700 ℃, while the structure with and without a ZnO seed layer were both considered. The magnetic and structural properties of $Zn_{0.95}Mn_{0.05}O$ nanorods has been characterized by X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDX), scanning electron microscopy (SEM), high-resolution transmission electron microscopy (HRTEM), and superconducting quantum interference device (SQUID). We demonstrate that the distribution and diameter of well-aligned $Zn_{0.95}Mn_{0.05}O$ nanorods are controllable, which strongly depend on the substrate temperature. Also, the magnetic properties are directly controlled by the morphologies of $Zn_{0.95}Mn_{0.05}O$ nanorods, and are thus appropriate for further applications.

MI-ThP5 Characterization of Metal Oxides Tunnel Barriers for use in a Non-Local Spin Detection Device, ***A. Matsubayashi***, College of Nanoscale Science and Engineering, the University at Albany-SUNY

Metal oxides can be utilized as interfacial layers between ferromagnetic metals and graphene to achieve spin injection into graphene. Utilizing the spin of the electron as well as its charge has the potential to be utilized for logic devices in the post CMOS era. The goal of our research is to inject and readout spins using a non-local measurement device. However the efficient spin injection has been realized its difficulty due to the conductivity mismatch problem1,2. In order to achieve the efficient spin injection, it has been determined that the insertion of a few nanometers of a tunnel barrier between the ferromagnetic metal and the graphene increases the contact resistance and measured spin lifetime3. However, non-uniformity of the tunnel barriers (pinholes)4 lowers the quality of the interface barrier. In this study, we investigate the fabrication of tunnel barrier on graphene using various metal oxides such as aluminum oxide grown under UHV conditions directly on the graphene. Graphene samples were loaded into an ultrahigh vacuum MBE (Molecular Beam Epitaxy) machine. D esired thickness of metals were deposited from a Knudsen cell. Samples were then transferred back into the load lock and exposed to approximately 130 mTorr of pure O2 for 20 min. Several measurements were performed including scanning electron microscopy, X-ray photoelectron spectroscopy, and angle resolved XPS characterize the electrical and structural quality of the films and their suitability for to be utilized as a tunnel barrier in graphene spin measurements.

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MI-ThP6 *In Situ* Scanning Tunneling Spectroscopy on Ordered, Epitaxial $La_{5/8-x}Pr_xCa_{3/8}MnO_3$ Films, ***Z. Gai***, Oak Ridge National Laboratory, *M. Gao,* Chinese Academy of Sciences, *P.C. Snijders, H.W. Guo, T.Z. Ward,* Oak Ridge National Laboratory, *H.J. Gao,* Chinese Academy of Sciences, *J. Shen*, Fudan University, China

Scanning probe microscopy has been shown to be a potent tool to investigate the structural, electronic, magnetic properties as well as their spatial distributions of strongly correlated perovskite manganites. Differences in tunneling spectra were interpreted to originate from the metallic and insulating phases in the material. However, questions were raised and still remain whether SPM on manganites probes bulk characteristics or is limited to surface properties. Complicating factors in this discussion are that most scanning probe studies either were performed on rather rough or grainy (and thus not very well ordered) surfaces, or on surfaces that were contaminated due to exposure to ambient air. Such ill-defined surfaces exhibit many localized surface states that often give rise to non-equilibrium occupation of states, and associated artifacts in scanning tunneling spectroscopy (STS) data, often masking or overwhelming possible bulk contributions. However, an STM does probe the electronic structure at the surface and this can include both surface and bulk contributions. Therefore, even on ideally ordered surfaces such as *in situ* grown and studied epitaxial manganite films, it is still unclear whether surface states (or even surface ground states that are different from their bulk counterparts) that are induced by the broken symmetry of the surface will overwhelm the bulk contributions in STS. We report temperature dependent scanning tunneling spectra recorded on *in situ* grown, single crystalline epitaxial $La_{5/8-x}Pr_xCa_{3/8}MnO_3$ (x=0.3) (LPCMO) films with different thicknesses: 100 nm and 25 nm. On the 100 nm LPCMO film, the tunneling spectra show a higher metal-insulator transition temperature as compared to the 25 nm LPCMO film. Consistently, bulk transport data for the two thicknesses of LPCMO films also show different metal-insulator transition temperatures, thus revealing that tunneling spectroscopy on manganites is sensitive to the bulk electronic structure and not limited to surface effects.

This effort was supported by the US DOE Office of Basic Energy Sciences, Materials Sciences and Engineering Division, and Center for Nanophase Materials Sciences, through the Oak Ridge National Laboratory.

MI-ThP7 Promise of New Multiferroics: Synthesis and Characterization of Epitaxial $NiTiO_3$ Films, ***T. Varga***, *T. Droubay, M.E. Bowden, S.A. Chambers, B. Kabius, W.A. Shelton, P. Nachimuthu, 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 $MTiO_3$ (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 $NiTiO_3$ has been prepared in epitaxial thin film form, whose structure is very close to that predicted to be a multiferroic. The synthesis of such new epitaxial films, their full structural characterization along with our first-principles DFT calculations to predict the desired $NiTiO_3$ structure and its stability are reported .

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