Wednesday Afternoon, November 2, 2011

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-ofart 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 University, 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 upperdeck 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 noncollinear moments. Calculations are based on the Keldysh formalism in which the non-equilibrium Green functions are calculated within a tightbinding 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 abinitio 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].

[1] A. Fert et al, Mat. Sci. Eng. B, 84, 1 (2001); S. A. Wolf, Science, 294, 1488 (2001).

[2] J. C. Slonczewski, J. Magn. Magn. Mat. 159, L1 (1996); L. Berger, Phys. Rev. B 54, 9353 (1996).

[3] W. H. Butler et al, *Phys. Rev. B*, **63**, 054416 (2001); J. Mathon et al, *Phys. Rev. B*, **63**, 220403(R) (2001).

[4] I. Theodonis et al, *Phys. Rev. Lett.* 97, 237205 (2006); M. Chshiev et al. *IEEE Trans. Mag.* 44 (11) (2008); A. Kalitsov et al, *Phys. Rev. B* 79, 174416 (2009); S.-C. Oh et al, *Nature Physics* 5, 898 (2009).

[5] H. X. Yang et al, Appl. Phys. Lett. 96, 262509 (2010).

[6] L. E. Nistor et al, Phys. Rev B 81, 220407 (2010).

[7] A. Kalitsov et al, Phys. Rev. B 82, 094420 (2010).

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.

^{*} Postdoc Award Finalist

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 Ge1xMnx quantum dots (QDs) on Si (001) by molecular beam epitaxial codeposition, 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

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