Magnetic Interfaces and Nanostructures Division
Room A210 - Session MI+2D-WeM

Emerging Multifunctional Magnetic Materials I and Magnetocaloric Materials

Moderator: Greg Szulczewski, University of Alabama

8:00am **MI+2D-WeM1 Spin-dependent Electron Reflection at Materials with Strong Spin-orbit Interaction***, **Markus Donath**, C. Angrick, A. Reimann, C. Datzer, A. Blob,* Muenster University, Germany*; J. Braun,* LMU München,, Germany*; H. Ebert,* LMU München, Germany

The reflection of electrons at surfaces becomes spin dependent due to exchange interaction in the case of ferromagnets or due to spin-orbit interaction in the case of heavy elements. It can be used for spin-polarization analysis, e.g., in angle-resolved photoelectron spectroscopy in a single-channel mode or in multi-channel-mode detectors by using the scattering target as a spin-polarizing mirror. In addition, the understanding of the spin-dependent scattering properties provides information about the surface barrier. We present a combined experimental and theoretical study of the spin-dependent electron reflection at surfaces with strong spin-orbit interaction. We performed spin-dependent very-low-energy electron diffraction (VLEED) experiments on Au(111), Bi_2Se_3, and W(110) over a wide range of energies and angles of incidence. We derived maps for the reflectivity, the Sherman function, and the figure of merit and compare them with *ab-initio* calculations. In addition, we discuss possible working points for the use as scattering targets in spin-polarization analyzers.

8:20am **MI+2D-WeM2 Competitive and Cooperative Electronic States in $Ba(Fe_{1-x}T_x)_2As_2$***, Q. Zou, M. Fu, Z. Wu, L. Li, A.-P. Li, D.S. Parker, A. Safat,* ***Zheng Gai***, Oak Ridge National Laboratory

The electronic structure inhomogeneity in Ni, Co and Ni doped $BaFe_2As_2$ 122 single crystals are compared using scanning tunneling microscopy/spectroscopy (STM/S) at atomic level within the pure superconducting (SC) dome, coexisting of SC and antiferromagnetic (AFM) phase, and non-SC phase regions. K-means clustering statistic method is utilized to categorize the various nanometer-size inhomogeneous electronic states described here as 'in-gap', 'L-shape' and 'S-shape' states immersed into the SC matrix for Ni-and Co-doped 122, and L-shape and S-shape states into metallic matrix for Cr-doped 122. Although the relative percentages of in-gap, L-shape and S-shape states various in three samples, the total volume fraction of the three electronic states is quite similar, coincident with the electron ($Ni_{0.04}$ and $Co_{0.08}$) and hole ($Cr_{0.04}$) numbers doped into the 122 compound. By combining the volume fractions of the three states, local density of the states (LDOS), field dependent behavior and global properties in these three sets of samples, the in-gap state in SC crystals is confirmed as magnetic impurity state from Co or Ni dopants, the L-shape state is identified as the spin density wave (SDW) which competes with the SC phase, and the S-shape state is found to be another form of magnetic order which constructively cooperates with the SC phase rather than competing with it. The comparison of the vortex structures indicates that those inhomogeneous electronic states serve as pinning centers for stabilizing the hexagonal vortex lattice.

8:40am **MI+2D-WeM3 Microscopic Origin of High Temperature Magnetism in Multiferroic Superlattices $(LuFeO_3)_m/(LuFe_2O_4)_1$***, **Janice Musfeldt**, S. Fan, K.A. Smith,* University of Tennessee Knoxville*; H. Das, A.F. Rebola,* Cornell University*; B.S. Holinsworth,* University of Tennessee Knoxville*; J.A. Mundy,* University of California at Berkeley*; C. Brooks, M. Holtz,* Cornell University*; R. Ramesh,* University of California at Berkeley*; D.A. Muller, D.G. Schlom, C.J. Fennie,* Cornell University*; S.A. McGill,* National High Magnetic Field Laboratory **INVITED**

Multiferroics are fascinating materials in which ferroelectric and magnetic orders coexist and spatial inversion and time-reversal symmetries are simultaneously broken. Outstanding challenges that currently prevent widespread application in memory and logic devices as well as neuromorphic computing include requirements for (i) a large coupling coefficient and (ii) room temperature operation. The development of a homologous series of superlattices with formula $(LuFeO_3)_m:(LuFe_2O_4)_n$ offers a path forward, although questions still exist about the microscopic origin of the high-temperature magnetism and the nature of the charge ordering pattern. In order to resolve these issues and provide additional insight into how external stimuli like magnetic fields can control behavior, we combined optical spectroscopy, magnetic circular dichroism, and first principles calculations to reveal the response of the $(LuFeO_3)_m:(LuFe_2O_4)_n$ superlattice. Each of the unique iron centers has excitations at slightly different energies, so by analyzing features in the dichroic rotation - which are proportional to net magnetization - and the character of the optical hysteresis loops at these energies, we reveal the magnetic field - temperature (H - T) behavior and how spin in the $LuFe_2O_4$ layer is the most significant contributor to the overall magnetic response. We also find that trends in the coercive field can be interpreted in terms of how the exchange strength depends upon the Fe site. The techniques developed here open the door to the microscopic analysis of materials with multiple metal centers and strong charge, spin, orbital, and lattice entanglement.

9:20am **MI+2D-WeM5 Hidden Local Spin-polarized Electronic States investigated by Spin- and Angle-resolved Photoelectron Spectroscopy***, **Taichi Okuda**,* Hiroshima University, Japan **INVITED**

Spin-polarized electronic states caused by spin-orbit interaction (SOI) have been attracted much attention recently because of the potential application for next-generation spintronic devices. In order to realize spintronic devices for various applications, it is necessary to search various kinds of new materials and systems possessing spin-polarized states. Although it was believed that the breaking of structural inversion symmetry is necessary to emerge the spin-polarized electronic states by SOI, the possibility of spin-polarized states by the inversion symmetry breaking at the local structure of crystals has been suggested recently[1]. Since the spin-polarization of the local structure of the other side of the crystal is opposite to maintain the zero net spin-polarization of materials, it is difficult to observe the local spin-polarization by macroscopic measurement and the spin-polarized states are, so to speak, hidden states.

Spin- and angle-resolved photoelectron spectroscopy(spin-ARPES) is one of the most powerful tools to investigate the spin-polarized electronic states caused by SOI since it can measure directly the k-dependent spin-polarization of electrons in the crystal (= spin-resolved band structure). Recent realization of high-efficiency, high-resolution and three-dimensional vector analysis in spin-ARPES measurement and the characteristic of the moderate proving depth of photoemission process enabled to investigate such hidden spin-polarized states. In this talk, some examples of the observation of the hidden spin-polarized states of layered materials (MoS_2, $PtSe_2$, and $LaOBiSe_2$, etc.)[2-4] will be presented. The finding of new materials possessing hidden spin-polarized states largely expands the variety of spin-polarized materials and will contribute to the future application for the spintronic devices.

[1] X. Zhang, Q. Liu, J.-W. Luo, A. J. Freeman, and A. Zunger, Nat. Phys. **10**, 387 (2014).

[2] R. Suzuki, M. Sakano, Y. J. Zhang, R. Akashi, D. Morikawa, A. Harasawa, K. Yaji, K. Kuroda, K. Miyamoto, T. Okuda, K. Ishizaka, R. Arita, and Y. Iwasa, Nat. Nanotechnol. **9**, 611 (2014).

[3] W. Yao, E. Wang, H. Huang, K. Deng, M. Yan, K. Zhang, T. Okuda, L. Li, Y. Wang, H. Gao, C. Liu, W. Duan, and S. Zhou, Nat. Commun. **8**, 14216 (2017).

[4] S.-L. Wu, K. Sumida, K. Miyamoto, K. Taguchi, T. Yoshikawa, A. Kimura, Y. Ueda, M. Arita, M. Nagao, S. Watauchi, I. Tanaka, and T. Okuda, Nat. Commun. **8**, 1919 (2017).

11:00am **MI+2D-WeM10 Compositional Tuning of Magnetic Exchange Interactions and Interpretation of the Pressure Dependence of the Magnetic Curie Temperature in High Entropy Alloys.***, **Michael Mchenry**,* Carnegie Mellon University **INVITED**

Magnetocaloric effect (MCE) materials are of interest in a more efficient technology than conventional gas compression refrigeration.MCE cooling is environmentally friendly since ozone depleting refrigerants are not used. Critical rare earths metals (REs) and compounds have large MCE response and working temperatures near room temperature. However, their scarcity, high price and corrosion limit their use. Recently, transition metal based high entropy alloys (HEAs) are studied for MCE applications due to convenient tunability of Curie temperatures,use of inexpensive components and tuning of the breadth of the magnetic phase transformation by distributing pair-wise magnetic exchange interations on a single fcc crystalline lattice. I will present our understanding of Curie temperature, T_c, engineering in metals with direct exchange interactions as rooted in the famous Bethe-Slater curve semi-empirically derived from considerations of the chemical bond and the constraints of the Pauli exclusion principle.

The Bethe-Slater curve predicts the dependence of the magnetic exchange interactions on D/d where D is the transition metal interatomic spacing and d is the spatial extend of the magnetic d-orbitals. The Bethe-Slater curveguides alloy design to optimize T_c's through distribution of exchange

interactions in MCE HEAs. I will present results for the composition and pressure dependence of the Curie temperature along with Mossbauer spectra, for which the average hyperfine field is proportional to an average pairwise exchange interaction and by inference T_c. Within this formalism, we consider J(D/d), i.e. the exchange interaction(s) as a function of D/d the variable for which the Bethe-Slater curve is parameterized. The P-dependence of $T_c$will be interpreted for FeCoNiMnCu 5-component HEAs with a room temperature T_c.

11:40am **MI+2D-WeM12 Epitaxy of Novel $Co_{1.5}Ti_{0.5}FeGe$ Heusler Alloy Thin Films**, ***Shambhu KC***[1]*, R. Mahat, T.J. Evans, S. Budhathoki, G.J. Mankey, A. Gupta, P. LeClair,* The University of Alabama

While the half-metallic ferromagnets are considered ideal candidates to be used for efficient spintronics devices, a single-phase microstructure with promising half-metallic character is recently reported in a bulk $Co_{1.5}Ti_{0.5}FeGe$ Heusler alloy[1]. This alloy has Ti substitution for Co atoms in the parent $Co_2FeTiGe$ alloy, where the parent alloy does not exhibit half-metallic behavior[2]. However, the Ti substitution is useful not only to stabilize single-phase behavior but also to tune half-metallicity by the Fermi level shift. In this work, successful growth of epitaxial thin films of this novel $Co_{1.5}Ti_{0.5}FeGe$ alloy on a-plane sapphire and $MgAl_2O_4$(100) by using DC magnetron sputtering will be reported. In-situ reflection high energy electron diffraction shows that the films grow epitaxially with smooth surfaces. X-ray diffraction analysis confirms the epitaxial relation and lattice parameters within a few percent of the reported bulk value. Presence of finite size Laue oscillations in the XRD pattern and 0.035˚ full width at half maximum of rocking curve obtained in case of films grown on a-plane sapphire describe excellent quality of the films. The presence of superlattice peaks; (200) and (111), indicate a strong tendency to form the $L2_1$ structure. The degree of B2 ordering is estimated to be as high as 0.92 showing that intermixing between the atoms in the octahedral and tetrahedral sites is limited. Atomic force microscopy shows that the films grown on $MgAl_2O_4$(100) are atomically smooth with a rms roughness of 0.2 nm. Magnetic measurements of films grown at 800ºC show that the saturation magnetization is in close agreement with the bulk value. Angle-dependent magnetization measurements show the symmetry of the coercivity is consistent with a magnetocrystalline anisotropy. Temperature-dependent transport measurements show metallic behavior and an ordinary magnetoresistance as high as 1.55 % is obtained at 100 K. All the above results describe the feasibility of growing good quality epitaxial films of novel $Co_{1.5}Ti_{0.5}FeGe$ alloy with the structural and magnetic properties consistent with reported bulk properties.

1. KC et al., Tunable Properties and Potential Half-Metallicity in $(Co_{2-x}Ti_x)FeGe$ Heusler Alloys; an Experimental and Theoretical Investigation, submitted to Phys. Rev. Materials.

2. Kumar et al., First-principles Calculation and Experimental Investigations on Full-Heusler Alloy Co_2FeGe, IEEE Transactions on Magnetics 45, 3997 (2009).

12:00pm **MI+2D-WeM13 Spin Transport in NiO Measured with Ferromagnetic Resonance**, *G.J. Mankey, T.J. Evans, S. KC,* ***Arjun Sapkota****, T. Mewes,* The University of Alabama

Recently, a measured spin diffusion length of approximately 22 nm was reported for spin current transmission through polycrystalline NiO.[1] The diffusion length is inferred by referencing the effective Gilbert damping constant in NiO/$Fe_{20}Ni_{80}$ bilayers as a function of NiO and $Fe_{20}Ni_{80}$ thickness. We present results using a different approach to determine the spin diffusion length, using trilayers of $Fe_{20}Ni_{80}$/NiO/Pt with FMR measurements covering the frequency range of 4 GHz to 50 GHz. The Pt serves as a spin sink when deposited directly on $Fe_{20}Ni_{80}$ and strongly increases the effective damping parameter. With NiO between the Pt spin sink and the ferromagnetic $Fe_{20}Ni_{80}$, the increase in damping parameter is diminished, and the decay length is extracted from measurements as a function of NiO thickness. Our preliminary measurements show that the decay length is smaller than 15 nm consistent with a decay length of approximately 4 nm determined from inverse spin hall effect measurements of $Y_3Fe_5O_{12}$/NiO/Pt structures.[2] In addition, at lower FMR frequencies (4 GHz as compared to 22 GHz) multiple resonances are observed for polycrystalline NiO, suggesting that ferromagnetic impurities are present in the antiferromagnet.

Results for polycrystalline and epitaxial trilayers will be presented, showing the effect of processing conditions on the spin diffusion length. These measurements will be correlated with microstructural and morphological characterization of the samples.

References

1 Tetsuya Ikebuchi, Takahiro Moriyama, Hayato Mizuno, Kent Oda, and Teruo Ono, Appl Phys Express **11** (7), 073003 (2018).

2 Yu-Ming Hung, Christian Hahn, Houchen Chang, Mingzhong Wu, Hendrik Ohldag, and Andrew D. Kent, AIP Advances **7** (5), 055903 (2017).

[1] **Falicov Student Award Finalist**

Author Index

Bold page numbers indicate presenter