Tuesday Afternoon, October 26, 1999

Magnetic Interfaces and Nanostructures Technical Group
Room 618/619 - Session MI-TuA

Magnetic Spectroscopies

Moderator: S.D. Bader, Argonne National Laboratory

2:00pm **MI-TuA1 Electronic Structure of Single Crystal CrO@sub 2@, *C.B. Stagarescu,*** *X. Su, D.E. Eastman,* University of Chicago*; K.N. Altmann, F.J. Himpsel,* University of Wisconsin, Madison*; A. Gupta,* IBM T.J. Watson Research Center

CrO@sub 2@ was predicted to exhibit half-metallic behavior with 100% spin polarization for electrons at the Fermi level, making it an ideal spin-injector for spin-polarized tunnelling junctions. Recently, a spin polarization of 90% at the Fermi level has been measured with a superconducting point contact.@footnote 1@ We have determined the relevant electronic states using polarization-dependent X-ray absorption (XAS) from the Cr 2p and O 1s core levels into the Cr 3d and O 2p states near the Fermi level, by X-ray magnetic dichroism (XMCD) at these edges, and by spin-polarized photoemission measurements. A clear picture emerges from the O 1s absorption edge, where a sharp peak is observed at 529.2 eV, followed by two peaks at energies of 2.1 and 3.5 eV higher. The first peak is excited only by the electric field vector (E) in the a-b plane, implying O 2p orbitals lying in that plane. It also exhibits a positive XMCD signal, which demonstrates significant hybridization of these (O 2p@sub x@, 2p@sub y@) states with the magnetic Cr 3d states of t@sub 2g@ character that produce the expected 100% majority spin polarization at the Fermi level. The two upper peaks have the opposite polarization dependence, implying an orientation of their O 2p orbitals mainly along the c axis (2X increase in magnitude from E parallel to the a axis to E perpendicular to the a axis, compared to a 10X decrease for the first peak). XMCD spectra obtained with magnetization along the easy (c) and hard (a) axis are compared. The consequences of these results for current models of the electronic structure are discussed. @FootnoteText@ @footnote 1@ R. J. Soulen et al, Science, 282, 85 (1998).

2:20pm **MI-TuA2 Underlying Simplicity of Magnetic Dichroism in the Photoelectron Spectroscopy of Gd*, J.G. Tobin,*** *S.R. Mishra,* Lawrence Livermore National Laboratory*; T.R. Cummins, G.D. Waddill,* University of Missouri, Rolla*; G. van der Laan,* Daresbury Laboratory, UK

Despite severe complexity in the 'raw' spectra of the Gd 5p's, the linear dichroic differences from remanently magnetized Gd/Y exhibit a startling underlying simplicity and consistency. The Gd 5p peaks display a strong cross sectional increase due to 'resonant photoemission' in the photon energy range of 135 to 150 eV. To properly model the pairs of 'raw' spectra acquired in linear dichroism experiments, an atomic model including multielectronic effects such as orbital momentum coupling is required. [1] However, the difference spectra obtained from the pairs are remarkably simple and consistent, in both experiment and atomic simulations. The development of a simplified one-electron picture to analyze the dichroic differences will also be discussed. S.R. Mishra, T.R. Cummins, G. D. Waddill, W.J. Gammon, G. van der Laan, K.W. Goodman, and J.G. Tobin, 'On the Nature of Resonant Photoemission in Gd,' Phys. Rev. Lett., 81, 1306 (1998).

2:40pm **MI-TuA3 Element-Resolved Magnetism Using Core-Resonant Magneto-Optical Techniques*, J.B. Kortright,*** *S.-K. Kim,* Lawrence Berkeley National Laboratory **INVITED**

Most magnetic films of current interest involve multiple magnetic species either homogeneously or heterogeneously distributed in single or multiple layers; examples include alloy or compound thin films, exchange-coupled layers or phases, and interfacial magnetism. A variety of soft x-ray magneto-optical techniques can resolve the aggregate magnetic response of such materials into that of the individual magnetic constituents, thereby offering opportunities to obtain a more detailed microscopic understanding of the macroscopic properties of interest. We have been extending traditional photon-based magneto-optical techniques, embodied in the complex Faraday and Kerr effects, from the near-visible regions into the soft x-ray range containing core levels of the 3d transition metals with associated large resonances in magneto-optical properties. Measuring the polarization of transmitted and reflected beams, in addition to their intensity, provides information that can, e.g., determine elemental moments both longitudinal and transverse to the propagation direction. In addition to field-dependent element-resolved information (hysteresis loops), spatial information both laterally and in depth on the nanometer scale and up is available from scattering and microscopy. Examples of the application of these techniques to better understand questions in exchange-coupled layers and alloy films will be given. @FootnoteText@ This work was supported by the Director, Office of Energy Research, Office of Science, Materials Sciences Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

3:20pm **MI-TuA5 Interatomic Effects in Resonant Photoemission in Fe/Cr Alloys and Bilayers*, E. Arenholz,*** Lawrence Berkeley National Laboratory*; A.W. Kay, C.S. Fadley,* Lawrence Berkeley National Laboratory and Univ. of California, Davis

Recently, first measurements and theoretical calculations of an interatomic multi-atom resonant photoemission effect (MARPE) have been reported by our group in measurements on several magnetic metal oxides (Science 281, 679 (1998)). MARPE occurs when the photon energy is tuned to a core-level absorption edge of an atom neighboring the emitting atom, with the photoemitting level having a lower binding energy than the resonant level; the resonant excitation is then found to significantly increase the photoemission intensity. We have now observed such effects in Fe/Cr alloys and bilayers. E.g. in Fe@sub 0.5@Cr@sub 0.5@, the Cr 2p intensity is enhanced by 20% when the photon energy is tuned to the Fe L@sub 3@ edge. Since MARPE is an interatomic effect the resonant enhancement of the Cr intensity in Fe/Cr alloys is expected to scale linearly with the number of Fe near neighbors. Although a monotonic decrease in the MARPE effect in Cr with decreasing Fe concentration is indeed found, deviations from the linear relationship expected from random mixing of Fe and Cr are observed. These findings will be discussed in terms of possible compositional clustering in Fe/Cr alloys, including additional data from Fe/Cr bilayers that were used to estimate the sensing length of the MARPE effect in this system. First observations of magnetic circular dichroism in the effect will also be presented.

3:40pm **MI-TuA6 Dispersions of Metallic Quantum Well States in the Cu/fccM(100) [M = Ni, Co, Fe] Systems*, A.G. Danese,*** *R.A. Bartynski,* Rutgers University

The study of the electronic properties of nonmagnetic/ferromagnetic bi-layers is essential to understanding the phenomenon of oscillatory magnetic coupling that is seen in magnetic multilayers. Using a phase accumulation model, we have calculated the dispersions of metallic quantum well (MQW) electronic states along @GAMMA@-barX-bar in the systems Cu/fccM(100) where M = Ni, Co, Fe. The model predicts that MQW states disperse with a high effective mass in regions of the 2-dimensional Brillouin zone where projected band gaps occur in the ferromagnetic material. Such regions occur near the belly and neck of the Cu Fermi surface. Near the belly, the regions of high effective mass will be observed below the Fermi energy (E@sub F@) for all three systems. Flat dispersions near the neck will occur about 1eV below the Fermi energy for Ni, about 1eV above E@sub F@ for Fe, and will pass through E@sub F@ for Co. These calculations give a good account of direct and inverse photoemission measurements from Cu/fccCo(100). We have recently performed inverse photoemission on Cu/fccFe(100) and Cu/fccNi(100) and the dispersions of the MQW states in these systems will be discussed and compared with the predictions of the phase accumulation model. Furthermore, there is evidence of parallel, flat MQW bands both below and above the Fermi level in the hybrid Cu/Fe/Cu/Ni system which indicate a possible optical resonance. This work was funded by the NSF, grant no. DMR98-01681 and the Petroleum Research Fund, grant no. ACS-PRF-33750-AC6,5.

4:00pm **MI-TuA7 Photoemission Study of Pseudomorphic Fe@sub x@Ni@sub 1-x@ and Co@sub x@Ni@sub 1-x@ Films on Cu(100)*, M. Hochstrasser,*** The Pennsylvania State University, U.S.*; N. Gilman, R.F. Willis,* The Pennsylvania State University*; F.O. Schumann, J.G. Tobin,* Lawrence Livermore National Laboratory*; E. Rotenberg,* Lawrence Berkeley National Laboratory (Advanced Light Source)

The k-space electronic structure of Fe@sub x@Ni@sub 1-x@ and Co@sub x@Ni@sub 1-x@ alloy films epitaxially grown on Cu(100) has been investigated with changing stoichiometry in angle-resolved photoemission and is compared to the electronic structure of fcc films of Co and Ni, as well as of Cu. We have monitored changes in the Fermi surface with changing stoichiometry and changing magnetic behavior. In the bulk, the magnetic moment deviates strongly from the Slater-Pauling curve at an Fe concentration of 65%, dropping quickly to zero as does the Curie temperature, at which point a structural phase transition from fcc to bcc is observed. Recently, it has been shown that Fe@sub x@Ni@sub 1-x@ films can establish in the fcc phase when grown as ultrathin films on Cu(100).@footnote 1@ The fcc to bcc structural transformation is quenched, but the magnetic instability persists. Furthermore, we

investigated with spin-resolved photoemission spectroscopy the regions relevant for the magnetic coupling with changing composition in Fe@sub x@Ni@sub 1-x@ films on Cu(100). We adress the questions: 1. Is there a relationship between the electronic structure and the sudden change in magnetization at a critical composition? 2. How does the Fermi surface evolve in these pseudomorphic alloy films? 3. What is the polarization of the states thought to be responsible for the oscillatory exchange coupling? The measurements show that the sp-band is a prominent feature of the Fermi surface throughout k-space for all of these alloys. A band structure calculation of Ni allows us to identify d-hole pockets arising from holes in the d-band(s) increasing with changing stoichiometry. The states thought to be responsible for the oscillatory exchange coupling, giving rise to giant magentoresistance (GMR) effects, are identified. @FootnoteText@ @footnote 1@ F. Schumann et. al., Phys. Rev. B, 56, 2668 (1997).

4:20pm **MI-TuA8 Magnetic Properties of Fe-based Alloys***, F.O. Schumann, J.G. Tobin,* Lawrence Livermore National Laboratory

The magnetic properties of fcc Fe@sub x@Ni@sub 1-x@ and Fe@sub x@Co@sub 1-x@ alloys grown on Cu(100)were investigated in an element-specific fashion.The technique employed was linear dichoism in photoemission (MLDAD), which by varying the chirality can also determine the magnetization axis. We observed a different behavior for the two alloys at Fe concentrations above 60%. At this concentration the Fe@sub x@Ni@sub 1-x@ alloy shows a strong reduction of the Fe dichroism associated with the invar instability.@footnote 1@ This is in contrast to the Fe@sub x@Co@sub 1-x@ alloy, where the Fe dichroism stays essentially constant across the concentration.This would indicate that a volume-moment instability is absent, which disagrees with a recent theoretical study.@footnote 2@ Despite these differences both systems show a change of the easy axis at roughly the same electron count.For small Fe concentrations the easy axis is in-plane along the [110] direction. This changes into the [100] direction at Fe@sub 60@Ni@sub 40@, which is at 0.8 excess electrons per atom when compared with Fe.This is different to the bulk, where a change occurs at Fe@sub 35@Ni@sub 65@. We find the easy axis change for Fe@sub x@Co@sub 1-x@ to occur at 35% Fe. This would be equivalent to 0.65 excess electrons when compared with Fe. @FootnoteText@ @footnote 1@ F.O. Schumann et al., Phys. Rev. Lett 79,5166 (1997). @footnote 2@ P.James et al., Phys. Rev. B 59,419 (1999).

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