MA 11: Magnetic Materials

Time: Monday 15:15–19:15 Location: HSZ 103

MA 11.1 Mon 15:15 HSZ 103

Magnetic properties of fcc Ni-based transition metal alloys — •Josef Kudrnovsky[1], Vaclav Drchal[1], and Patrick Bruno[2] — [1]Institute of Physics AS CR, Prague — [2]ESRF, Grenoble

Electronic properties and finite-temperature magnetism of Ni-based transition metal alloys with the face-centered cubic structureis are studied theoretically by ab initio calculations. While the calculated total and local magnetic moments agree well with the experiment, the evaluation of the Curie temperature from first-principles represents much more delicate problem. The mean-field approximation, the random-phase approximation (RPA), as well as the renormalized RPA by Bruno extended to random alloys were tested, the latter giving the most satisfactory agreement with the experiment for a broad class of Ni-based alloys of the type Ni(1-x)M(x) (M=Cu, Pd, Co, Fe, and Mn) over the whole concentration range.

We will also discuss differences between fcc-phases and artificially prepared bcc-phases of Ni and Permalloy.

MA 11.2 Mon 15:30 HSZ 103

Electronic and magnetic properties of Gd-based materials: Beyond the LDA — •Samir Abdelouahed[1], Mebarek Alouani[2], and Jürgen Henk[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Institut de Physique et de Chimie des Matériaux de Strasbourg (IPCMS), France

The FLAPW method has been used to study the electronic structure of gadolinium-based materials. The 4f electron-electron interaction was treated by the LDA+U method to improve the description of electronic and magnetic properties. For gadolinium, x-ray absorption spectroscopy (XAS) and x-ray magnetic circular dichroism (XMCD) spectra calculated including U agree better with experiment, as compared to those of the standard LDA (GGA) treatment. Furthermore, the XMCD spin and orbital moments, obtained from the sum rules, compare favorably to the self-consistent results.

The tiny magnetocrystalline anisotropy energies (MAE's) of bulk Gd, GdN, and GdFe2 have been calculated by means of the magnetic-force theorem. The energy position of the 4f-state affects significantly the MAE's. For example, the magnetic anisotropies in GGA and in GGA-core calculations are factors of about 10 and 3 larger than that of the GGA+U approach, indicating the importance of hybridization in these systems.

MA 11.3 Mon 15:45 HSZ 103

Spin freezing and slow magnetization dynamics in geometrically frustrated magnetic molecules with exchange disorder — •Christian Schröder[1,2], Yuji Furukawa[2], Marshall Luban[2], Ruslan Prozorov[2], and Ferdinando Borsa[2,3] — [1]Department of Engineering and Mathematics, University of Applied Sciences Bielefeld, D-33602 Bielefeld, Germany — [2]Ames Laboratory & Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — [3]Dipartimento di Fisica "Alessandro Volta", Università di Pavia, I-27100 Pavia, Italy

We show that intramolecular exchange disorder recently found in the geometrically frustrated magnetic molecules $\{Mo_{72}Fe_{30}\}$ and $\{Mo_{72}Cr_{30}\}$ leads in a classical Heisenberg model description to spin freezing and slow magnetization dynamics reminiscent of spin glass behavior. Our low temperature and low magnetic field NMR measurements on these molecules are explained as a cross-over of the proton line width from paramagnetic behavior to a frozen spin configuration at about 400 mK.

MA 11.4 Mon 16:00 HSZ 103

Anisotropic magnetoresistance (AMR) of magnetic graphite — •Jose Barzola-Quiquia, Pablo Esquinazi, Daniel Spemann, and Tilman Butz — Institut für Experimentelle Physik II, Universität Leipzig, D-04103 Leipzig

Complementing the experimental evidence for the existence of magnetic order induced by proton irradiation in graphite obtained by XMCD, SQUID, and LEμSR, we studied in this work the magneto-transport of irradiated oriented graphite samples. The resistance measured for fields applied parallel to the planes and at different angles respect to the current shows the typical behaviour of the AMR observed in ferromagnets including irreversibility loops. The results confirm the existence of magnetic order in irradiated graphite and rule out magnetic impurities as origin, in agreement with XMCD and LEμSR results.

MA 11.5 Mon 16:15 HSZ 103

Magnetoresistance and magnetoimpedance measurements on iron whiskers — •Matthäus Langosch, Haibin Gao, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, 66123 Saarbrücken, Germany

Magnetoimpedance (MI) measurements on iron single crystals (iron whiskers) with growing directions <100> and <111> were carried out at room temperature as a function of applied longitudinal magnetic field, current amplitude and frequency. Simultaneous Kerr microscopy was employed to study the magnetic surface domain structure of the samples. Measurements also provide ordinary magnetoresistance (MR) contributions. The contributions of the MI and MR effects were discussed based on the experimental results. The correlation between domain structure and magnetoimpedance effect was studied on the basis of Kerr microscopy images and resistivity data.

MA 11.6 Mon 16:30 HSZ 103

Semiconducting and half-metallic ternary rare earth compounds — •Frederick Casper and Claudia Felser — Institute of Inorganic and Analytical Chemistry,

Rare earth compounds with the LiAlSi and LiGaGe structure types have been investigated by means of band structure calculations. The LiAlSi structure type is more familiarly known as the half-Heusler structure type, whereas LiGaGe is a closely related hexagonal variant. Both structure types can be found within the same REYZ series, depending on the size of the RE element and the Y - Z bond length. A remarkable feature of some REYZ half-Heusler compounds with 18 valence electrons is that despite being composed of only metallic elements, they are semiconductors. Calculated band gaps, in comparison to experimental ones, are frequently too large, which can be attributed to some finite site disorder in the compounds. LiGaGe compounds have an additional degree of freedom, namely the degree of puckering of the layers. These compounds can become semiconducting at a certain value of puckering. Half-metallic behaviour is rarely found in this structure type. This work is supported by by DfG grant FE633/1-1 within SPP1166.

MA 11.7 Mon 16:45 HSZ 103

Effects of film thickness and Co doping on the magnetism of Pd structures — •Volker Pankoke and Gemming Sibylle — FZD,Desden,Germany

Palladium in its ground-state has a non magnetic fcc structure. We suggest that it can be forced to get ferro-magnetic by an expansion of the lattice constant, or in case of thin films by a varying number of atomic layers. Another option to induce magnetism is to dope the Pd structures with 3d transition metals. We used first principles methods to calculate the magnetization density of different Co doped and undoped Pd structures. Calculations were carried out with the projector augmented waves (PAW) method in the LDA+U approximation and a plane wave basis set. In addition the linear augmented plane waves (LAPW) method was used and compared with the PAW results. Both methods show, that doping with 3d transition metals leads to magnetic moment at the Pd sites of the crystal. In case undoped Pd films the PAW results are similar to existing LAPW calculations.

MA 11.8 Mon 17:00 HSZ 103

Interaction Domains in High Performance NdFeB Thick Films — •Tom Woodcock[1], Kirill Khlopkov[1], Arno Walther[2,3], Nora Dempsey[2], Dominique Givord[2], Ludwig Schultz[1], and Oliver Gutfleisch[1] — [1]IFW Dresden, IMW, P.O. Box 270116, 01171 Dresden, Germany — [2]Insitut Néel, CNRS-UJF, 25 ave. de Martyrs, 38042, Grenoble, France — [3]CEA Léti - MINATEC, 17 rue des Martyrs, 38054 Grenoble, France

Thick sputtered films (5-300 micron) of NdFeB have excellent hard magnetic properties which make them attractive for applications in micro-electro-mechanical systems (MEMS). A two step process consisting of triode sputtering and high temperature annealing produced films with energy densities approaching those of sintered NdFeB mag-

nets.

Magnetic force microscopy (MFM) using hard magnetic tips showed that the films deposited without substrate heating and at 300°C exhibited magnetic domains typical of low anisotropy materials. These films were amorphous in the as-deposited state. The film deposited at 500°C was crystalline and displaid hard magnetic properties. This was reflected in the magnetic microstructure which showed interaction domains typical of highly textured and high magnetic anisotropy materials with a grain size below or equal to the critical single-domain particle limit. With increasing substrate temperature, the domain patterns of the annealed films became coarser, indicating higher degrees of texture.

15 min. break

MA 11.9 Mon 17:30 HSZ 103

Hard X-ray Standing Wave Photoemission from Multilayer Nanostructures. — •Christian Papp[1], Benjamin Balke[1], Shigenori Ueda[2], Hideki Yoshikawa[2], Shao Long He[2], Keisuke Kobayashi[2], Guiseppina Conti[3], Daniel Buergler[4], Claus Schneider[4], Sven Doering[5], Ulf Berges[5], Carsten Westphal[5], and Charles S. Fadley[1] — [1]Lawrence Berkeley National Laboratory, CA, USA — [2]SPring 8, Japan — [3]Applied Materials, CA, USA — [4]Forschungszentrum Juelich — [5]Lehrstuhl für Physik E1, Uni Dortmund

We have used x-ray standing wave excitation of photoelectrons to study buried layers and interfaces in multilayer nanostructures. In particular, measurements carried out at SPring 8 with 6 keV photon energy will be emphasized. The samples were grown on synthetic multilayer mirrors and the x-ray incidence angle was tuned to the 1st order Bragg reflection. Scanning angle, photon energy, or distance along a wedge profile in the sample permits scanning the resultant standing wave field through nm-scale structures and analyzing the depth distribution of their structural, chemical, electronic, and magnetic properties. Using hard x-ray excitation permits via the higher kinetic energy of the electrons studying those properties at greater depths. The systems discussed will be related to integrated circuit production (titanium nitride on silicon) and to a magnetic tunnel junction (in particular, the electronic properties of the Fe/MgO interface).

MA 11.10 Mon 17:45 HSZ 103

Coupling between Ho and Cr magnetic sub lattice in rare-earth orthochromite HoCrO3 — •Naveen Kumar Chogondahalli M.[1], Yinguo Xiao[1], Yixi Su[2], Jörg Persson[1], Anatoliy Senyshyn[3], and Thomas Brückel[1,2] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Centre for Neutron Science, IFF, Forschungszentrum Jülich, Outstation at FRM II, 85747 Garching, Germany — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), 85747 Garching, Germany

HoCrO3 crystallizes in orthorhombic structure with the space group Pbnm in the temperature range 4 to 300 K. Both the magnetization and heat capacity measurements clearly indicate the onset of magnetic ordering at TN =140 K. From Curie-Weiss fit of magnetic susceptibility, the Curie temperature is found to be -28.81 K and the effective moment, Peff = 15.78 bohr magneton. The temperature dependence of magnetic structure is investigated by using the neutron powder diffraction. Below Neel temperature Cr3+ orders antiferromagnetically with the moments aligned along c-axis. The canted ferromagnetic ordering of Ho3+ with moments aligned perpendicular to Cr3+ moments is observed at lower temperatures. The molecular field of Cr cancels at Ho site. It is likely that the ordering of Ho is induced by the fluctuations of Cr subsystem magnetization but not by magnetization itself. This may be order by disorder type of induced ordering [J. Villain et al., 1980]. Such an ordering is only possible if the resulting interactions, Cr-Ho is much stronger than Ho-Ho antiferromagnetic exchange.

MA 11.11 Mon 18:00 HSZ 103

Hyperfine magnetic field on iron atoms as indication of stoichiometry in Co_2FeSi — •Vadim Ksenofontov[1], Benjamin Balke[1], Claudia Felser[1], Marek Wójcik[2], Sabine Wurmehl[3], Horst Schneider[4], and Gerhard Jakob[4] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg-University, 55099 Mainz, Germany — [2]Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warszawa, Poland — [3]Department of Applied Physics, Physics of Nanostructures, Eindhoven University of Technology, PO Box 513, 5600 MB Eindhoven, The Netherlands — [4]Institute of Physics, Johannes Gutenberg - University, 55099 Mainz, Germany

The Heusler compound Co_2FeSi is a promising half-metallic material for thin films spintronic applications. Among the factors reducing spin-polarization, the defects and antisite disordering in such materials play a crucial role. To clarify effects of the non-stoichiometry, the continuous series of model solid solutions $Co_{3-x}Fe_xSi$ ($0.96 < x < 1.4$) was investigated by ^{57}Fe Mössbauer spectroscopy and ^{59}Co nuclear magnetic resonance. It has been shown that hyperfine magnetic fields on Fe can be used to monitor a non-stoichiometry in Co_2FeSi-based bulk samples and thin films.

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MA 11.12 Mon 18:15 HSZ 103

Strain induced magnetism in La0.5Ca0.5MnO3 systems — •Thomas Tietze[1], Daniela Nolle[1], Gisela Schütz[1], Eberhard Goering[1], Gülgün Aydogdu[2], and Hanns-Ulrich Habermeier[2] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

The La1-xCaxMnO3 exhibits, besides the double exchange relate magneto resistive effects, many interesting properties as a function of the doping level. Depending on the doping level x the system may exhibit ferromagnetism, antiferromagnetism, orbital ordering, and charge ordering. Epitaxial tensile and compressive strains are very important for the fine tuning of the lattice degree of freedom and therefore for the magnetic nearest neighbor coupling. By *adjusting* tensile and compressive strain with corresponding substrates one can switch between FM and AFM coupling between the FM ordered ab-planes. In order to investigate the influence of different substrates and relaxation effects element specific XMCD measurements were performed on La0.5Ca0.5MnO3 systems.

MA 11.13 Mon 18:30 HSZ 103

Investigations on the MTJ interface Co_2MnSi-MgO using electron spectroscopy with x-ray standing wave excitation. — •Benjamin Balke[1], Christian Papp[1], Catherine A. Jenkins[2], Gerhard H. Fecher[2], Charles S. Fadley[1], and Claudia Felser[2] — [1]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [2]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany

We have used x-ray standing wave excitation of photoelectrons to study buried layers and interfaces in multilayer nanostructures. In particular, measurements carried out at the ALS with 1.2 keV photon energy will be emphasized. The samples were grown on synthetic multilayer mirrors and the x-ray incidence angle was tuned to the 1st order Bragg reflection. Scanning angle, photon energy, or distance along a wedge profile in the sample permits scanning the resultant standing wave field through nm-scale structures and analyzing the depth distribution of their structural, chemical, electronic, and magnetic properties. In this study we investigated the interface between the Heusler compound Co_2MnSi and MgO as used in MTJs. Therefore we used a wedge of Co_2MnSi with a MgO top layer and used photoelectron spectroscopy with X-ray standing wave excitations. B.B. and C.P. gratefully acknowledge the Feodor Lynen Fellowship by the Humboldt Foundation. Additionally, the authors gratefully acknowledge financial support by the DfG (Research Unit 559).

MA 11.14 Mon 18:45 HSZ 103

Polarized neutron scattering on geometrically frustrated magnets with Swedenborgite structure — •Martin Valldor[1], Yvonne Sanders[2], and Werner Schweika[2] — [1]II. Physikalisches Institut, Universität Köln, 50937 Köln, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

Diffuse scattering of polarized neutrons on cobaltate polycrystalline samples with Swedenborgite structure, ABaCo3BO7 (A = Y, Ca, and B = Co, Fe, Al, Zn) was used to study the change in magnetic order depending on chemical composition. The atomic structure contains alternate stacking of kagome and triangular layers of metal ions, all in tetrahedral oxygen coordination. Geometrical frustration of antiferromagnetically coupled spins should suppress long-range order even at low temperatures despite strong spin-spin coupling in the Swedenborgites. The diffuse magnetic scattering in Y0.5Ca0.5BaCo4O7 reveals two dimensional (2D) spin correlations on the kagome sublattices to-

wards the entropically favoured V3*V3 structure and suggests a decoupling of layers on triangular sites. Co-substitution by Al and Zn yields similar diffuse magnetic scattering, however, spin dilution results in even more disordered spin liquid or spin glass states. With B = Fe or Co, differences in the magnetic scattering evolve, indicating the onset of spin correlations perpendicular to the kagome layers.

MA 11.15 Mon 19:00 HSZ 103

Thermal stability and magnetic properties of Fe-Co-B-Si-Nb glassy alloys — •Mihai Stoica[1], Ran Li[1], and Jürgen Eckert[1,2] — [1]IFW Dresden, Institute for Complex Materials, P.O. Box 270116, D-01171 Dresden, Germany — [2]TU Dresden, Institute of Materials Science, D-01062 Dresden, Germany

The fully glassy rods of $[(Fe_xCo_{1-x})_{0.75}Si_{0.05}B_{0.25}]_{94}Nb_6$ alloys (x = 0.4, 0.5 and 0.6) in diameters up to 2 mm were produced by copper mold casting. The effect of Fe substitution in these glassy alloys on thermal stability and melting behavior were studied by differential scanning calorimetry. Phase evolution of the glassy alloys during heating crystallization process was evaluated using X-rays diffraction. The first crystallization stage results in the precipitation of metastable $(Fe,Co)_{23}B_6$ crystalline phase in the glassy alloys. The behaviour of the glassy alloys in DC applied field was investigated by means of vibrating sample magnetometer. The investigated samples are soft magnetic. Further, the influence of crystallization on the saturation magnetization (M_s), coercivity (H_c) and Curie temperature (T_c) were evaluated, which indicated that $(Fe,Co)_{23}B_6$ phase can improve the M_s and T_c, while also increase the H_c.