MA 28: Magnetic Materials

Time: Wednesday 15:00–18:00 Location: H22

MA 28.1 Wed 15:00 H22

Electronic Structure Calculations of Materials with Increased Magnetic Anisotropy Energies — •Alexander Edström, Olle Eriksson, and Jan Rusz — Uppsala University, Department of Physics and Astronomy, Division of Materials Theory, Uppsala, Sweden

Materials with a high saturation magnetization, as well as high magnetic anisotropy energy, are required to produce permanent magnets which are important in a wide range of applications. Here DFT calculations are used to study magnetizations and magnetic anisotropy energies in a variety of materials. Certain materials such as FeCo based alloys, with relatively large saturation magnetization, are found to also exhibit high magnetic anisotropy energies at particular crystal distortions and alloy concentrations [1]. This makes them potentially useful for permanent magnet applications. We report first principles calculations of magnetization and magnetocrystalline anisotropy energy for a wide range of concentrations and deformations of the cubic and hexagonal lattices. This work was supported by ERC project RE-FREEPERMAG and Swedish Research Council.

1. T. Burkert, et al, PRL 93, 027203 (2004)

MA 28.2 Wed 15:15 H22

Magnetism and structural instability in frustrated intermetallic AFe_4X_2 systems — •Inga Kraft, Christoph Bergmann, Katharina Weber, Nandang Mufti, Christoph Geibel, and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, Dresden

Frustration in intermetallic systems lead to an increase of quantum fluctuations and often result in unusual properties. Magnetic, thermodynamic, and structural data of the intermetallic AFe_4X_2 compounds (A=Sc,Y,Lu,Zr; X=Si,Ge) evidence that these compounds cover the whole regime from frustrated AFM order up to an AFM quantum critical point. In agreement with the experimental findings our DFT calculations yield an orthorhombic ground state and together with magnetic order a strong interplay of structure and magnetism. We discuss the influence of the A and X site atoms on the strength of magnetic interactions and the size of structural distortion.

MA 28.3 Wed 15:30 H22

Calculation of the angular dependence of XMLD in reflection in 3d transition metals at 3p edges — •Dominik Legut[1], Peter Oppeneer[2], Marc Tesch[3], Hans-Christoph Mertins[3], Markus Gilbert[3], and Andreas Gaupp[4] — [1]Nanotechnology Centre, Ostrava, Czech Republic — [2]Department of Physics and Astronomy, Uppsala, Sweden — [3]FH Münster, Steinfurt, Germany — [4]HZB, Berlin, Germany

The full angular dependence of the x-ray magnetic linear dichroism (XMLD) in reflection spectra on the crystalline orientation of the magnetization was investigated for ferromagnetic bcc Fe, fcc Ni and fcc Co. The anisotropic XMLD spectra were computed in the single electron picture within the framework of the DFT. The excitation stemming from semicore 3p levels were considered. The calculated results show similarities as well as differences between $L_{2,3}$ and $M_{2,3}$ edges, because of hybridization of two $3p_{1/2}$ sub-levels and four $3p_{3/2}$ sub-levels (m_j levels).[1] The XMLD signal is strongly dependent on the magnetization direction with respect to the crystal axes. Furthermore, the influence of the sample thickness on the reflection coefficients is investigated. The magnitude of the lattice distortion vs. the influence of the spin-orbit coupling on the reflection coefficients for general magnetization direction is revealed. The calculated data show very good agreement with recently recorded spectra of bcc Fe. The influence of the spin-orbit coupling and exchange interaction at 3p states is revealed.

References:

1. S. Valencia *et al.*,Phys. Rev. Lett. **104**, 187401 (2010).

MA 28.4 Wed 15:45 H22

Quadratic magneto-optical permittivity coefficiets in cubic Fe, Co, Ni calculated ab-initio — Jana Hamrlova, •Jaroslav Hamrle, Dominik Legut, Kamil Postava, and Jaromir Pistora — Nanotechnology Centre, VSB - Technical University of Ostrava, Czech Republic

Using ab-initio calculations, we determine spectra of the second-order magneto-optical permittivity coefficients (G_{44}, ΔG) for ferromagnetic bcc Fe, fcc Ni and fcc Co. Those second-order magneto-optical permittivity coefficients provide phenomenological description of all second-order magneto-transport effect, such as AMR, quadratic MOKE, XMLD, magneto-refracticity, etc. depending on the investigation technique and the energy of the probing photon (zero photon energy means dc). The calculations of the conductivity/permittivity tensor elements are done within the framework of DFT using general magnetic orientation with respect to the crystal axis. Then, dependence of the permittivity elements on general magnetization orientation is compared with expected dependences as provided by symmetry arguments.

MA 28.5 Wed 16:00 H22

First-pinciples calculations of Gilbert damping parameter for magnetic metals and alloys — •Sergiy Mankovsky, Diemo Koedderitzsch, and Hubert Ebert — Dept. Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Germany

The results of first-principles calculations of the elements of the Gilbert damping tensor, $\alpha_{\nu\nu}$, are presented. Calculations have been performed for various systems, e.g., pure 3d transition metals, magnetic alloy systems and magnetic semiconductors. The anisotropy of the Gilbert damping and its dependence on the orientation of the magnetization and structure parameters, have been analyzed. Furthermore, the role of chemical and temperature induced structural and magnetic disorder has been investigated. The corresponding scattering mechanisms have been accounted for by using the coherent potential approximation (CPA) alloy theory. The theoretical results for the Gilbert damping parameters are compared with available experimental data.

MA 28.6 Wed 16:15 H22

Partial substitution of Nd in FeNdB permanent magnets by economic rare earth metals — •Dagmar Goll[1], Ralf Löffler[1], Arne Huber[2], and Gerhard Schneider[1] — [1]Hochschule Aalen, Institut für Materialforschung, Aalen — [2]Robert Bosch GmbH, Gerlingen-Schillerhöhe

High-performance permanent magnets like Fe-Nd-B sintered magnets are very promising for high-power motor and generator applications in resource efficient mobility and renewable energy. However, the associated increasing demand for intermetallic rare earth (RE) and transition metal (TM) compounds recently gets somewhat abated due to the dependence on rare earth metal raw materials from China. Partial substitution of Nd by economic RE metals like Ce, La or Y may result in more cost-efficient magnets. To evaluate the optimum conditions for realizing cost-efficient high-performance magnets the intrinsic magnetic properties (anisotropy constant K_1, saturation polarization J_s) of as-cast $Fe_{14}(Nd_{1-x}RE_x)_2B$ are determined from Kerr microscopy investigations and magnetometry measurements of the corresponding hysteresis loops *(project supported by BMBF).*

15 min. break

MA 28.7 Wed 16:45 H22

Ab initio study of thermodynamic, electronic, magnetic, structural, and elastic properties of Ni_4N allotropes — Pavlina Hemzalova[1,2,3], •Martin Friak[1,3,4], Mojmir Sob[2,3,4], Alexander Udyansky[1], Duancheng Ma[1], and Joerg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Masaryk University, Brno, Czech Republic — [3]Central European Institute of Technology, CEITEC MU, Brno, Czech Republic — [4]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic

We have used density functional theory calculations to study thermodynamic, structural, elastic, and electronic properties of Ni_4N, that forms e.g. when nitriding Ni-containing alloys, in eight different crystallographic phases. In agreement with the experimental findings, the cubic structure with Pearson symbol cP5, space group Pm-3m (221), is found to be the most stable. We determine structural parameters, internal degrees of freedom, bulk moduli and their pressure derivatives for all eight allotropes. The thermodynamic stability and bulk modulus is shown to be anti-correlated. Comparing ferromagnetic and non-magnetic states, we find common features between the magnetism of

elemental Ni and studied ferromagnetic Ni_4N structures. For cubic allotropes, we predict single-crystalline elastic constants, their area moduli, and homogenized polycrystalline elastic moduli. We demonstrate that the elastic anisotropy of the ground-state Ni_4N is qualitatively opposite to that in the elemental Ni. One of the studied metastable cubic phases is found auxetic, i.e. exhibiting negative Poisson ratio.

MA 28.8 Wed 17:00 H22

Contributions of domain wall substructures to the magnetization configurations — •Sukhvinder Singh, Haibin Gao, and Uwe Hartmann — Experimental Physics, Saarland University, P O. Box 151150, D-66041, Saarbrücken, Germany

Magnetic domain wall substructures have strong influences on domain wall behavior, i.e., movement and pining effects within an external magnetic field. In this work, contributions of domain wall substructures (Bloch lines, cross-tie wall components, vortex-antivortex pairs) and individual vortices to the magnetization configurations of EBL-patterned Permalloy thin films and Fe-whiskers have been investigated. MFM was employed to check the influence of those substructures' interactions with notches and sample edges with and without an in-plane static magnetic field. The result shows the attractive interaction between magnetic charges at the edge and the vortex-antivortex dipolar charges in the cross-tie wall. Stripe domains were observed for films of more than 100 nm of thickness. In contrast, well arranged stripe domains mixed with Landau domain pattern or cross-tie wall structures were found on thinner samples. OOMMF was used to model the behavior observed by MFM.

MA 28.9 Wed 17:15 H22

Spectroscopic study of the Kondo semiconductors CeM_2Al_{10} (M = Ru, Os and Fe) — •Fabio Strigari[1], Thomas Willers[1], Zhiwei Hu[2], Chang-Yang Kuo[2], Stefano Agrestini[2], Andrea Severing[1], and Liu Hao Tjeng[2] — [1]Institute of Physics II, University of Cologne — [2]MPI for Chemical Physics of Solids, Dresden

The orthorhombic CeM_2Al_{10} compounds with M = Ru, Os, and Fe belong to a fairly new family of Ce Kondo semiconductors, which exhibit a novel magnetic phase transition at $T_0 = 27\,K$ (M = Ru) and 29 K (M = Os). The ordering mechanism is still a matter of debate since the ordering temperature is unexpectedly high and the ordered moment strongly reduced. The isostructural $CeFe_2Al_{10}$ lacks any phase transition and shows the highest degree of hybridization between $4f$ and conduction electrons within the family. For $CeRu_2Al_{10}$ and $CeOs_2Al_{10}$ the static magnetic susceptibility shows a strong anisotropy and Curie-Weiss behavior down to T_0 and 40 K, respectively, whereas for $CeFe_2Al_{10}$ it suggests more intermediate valent behavior. Due to the presence of the crystalline electric field, the $4f$ ground state wave functions are expected to be highly anisotropic and their knowledge is essential to understand the magnetic properties in this compounds.

We performed extensive experimental studies by means of x-ray based spectroscopic techniques – namely soft x-ray absorption, resonant inelastic x-ray scattering and hard x-ray photoemission spectroscopy – in order to determine the crystal-field ground state and quantitatively analyze the $4f$ valence for the members of the 1-2-10 family.

MA 28.10 Wed 17:30 H22

Nature of local moments in La(Sr)CoO3 — •Jan Kunes and Vlastimil Krapek — Institute of Physics, AS CR, Prague, Czechia

We present a numerical study of magnetic properties of LaCoO3 and SrCoO3 using the dynamical mean-field theory. In particular, we investigate the origin of the local magnetic moments (Curie susceptibility). Using the decomposition of the temporal spin-spin correlation functions into contributions from atomic multiplets we generalize the notion of atomic multiplets to situations with the strong covalent bonding. We show that the magnitude of the local moment is in general not a good parameter to identify the microscopic atomic states underlying the formation of local magnetic moments. Our numerical results exclude the so called intermediate spin states to play an important role in magnetism of LaCoO3.

MA 28.11 Wed 17:45 H22

Investigation on magnetoacoustic properties of spin-ice materials Dy2Ti2O7 and Ho2Ti2O7 — •Salim Erfanifam[1], Sergei Zherlitsyn[1], Joachim Wosnitza[1], Roderich Moessner[2], Andrei Anatolievich Zvyagin[2,3], Paul McClarty[2], Oleg Petrenko[4], and Geetha Balakrishnan[4] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [2]Max-Planck Institut für Physik komplexer Systeme, D-01187 Dresden, Germany — [3]B.I. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, 61103, Ukraine — [4]University of Warwick, Department of Physics, Coventry CV4 7AL UK

We have investigated elastic properties of the spin-ice materials Dy2Ti2O7 (DTO) and Ho2Ti2O7 (HTO) for a wide range of temperature and magnetic field. Our studies of the sound characteristics for several acoustic modes evidence a renormalization of the sound velocity and the sound attenuation due to phase transformations at applied magnetic field as well as an interaction with low-energy magnetic excitations (topological defects). The most prominent anomalies are quasi-periodic peaks in the sound velocity and in the sound attenuation observed in DTO due to non-equilibrium processes arising in the external magnetic field. These results were analyzed theoretically using exchange-striction coupling, which shows a good agreement between theory and experiment. The obtained results at high magnetic fields exhibit some pronounced anomalies around 50 T for both compounds. Our calculations including crystal-electric field effects show satisfactory agreement with experiment.