MA 62: Disodered Magnetic Materials

Time: Friday 9:30–11:30 Location: HSZ 401

MA 62.1 Fri 9:30 HSZ 401

An ab initio study of magnetism in disordered Fe-Al alloys with thermal antiphase boundaries — •Martin Friák[1], Miroslav Golian[1], David Holec[2], Nikola Koutná[3], and Mojmír Šob[1] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Department of Materials Science, Montanuniversität Leoben, Leoben, Austria — [3]Institute of Materials Science and Technology, TU Wien, Vienna, Austria

We have performed a quantum-mechanical study of a disordered B2 phase of $Fe_{70}Al_{30}$ alloy with and without antiphase boundaries (APBs) with the {001} crystallographic orientation of APB interfaces. We used a supercell approach with the atoms distributed according to the special quasi-random structure (SQS) concept. Our study was motivated by experimental findings by Murakami *et al.* (Nature Comm. 5 (2014) 4123) who reported significantly higher magnetic flux density from A2-phase interlayers at the thermally-induced APBs in $Fe_{70}Al_{30}$ and suggested that the ferromagnetism is stabilized by the disorder in the A2 phase. Our computational study confirms this suggestion (Friák *et al.* (2019), submitted to Nanomaterials) and explains details of the underlying mechanism. The Fe atoms in the A2 phase have the average magnetic moment by 17.5 % higher than in the B2 phase. We link the changes in the magnetism to the fact that the Al atoms in the first nearest neighbor shell of Fe atoms nonlinearly reduce their magnetic moments (M. Friák and J. Neugebauer, Intermetallics 18 (2010) 1316). Lastly, our atomistic simulations of sharp APBs confirmed a temperature-dependent formation of the A2-phase interlayers.

MA 62.2 Fri 9:45 HSZ 401

Variation of open volume defects during magnetic phase transitions — •Maciej Oskar Liedke[1], Maik Butterling[1], Jonathan Ehrler[1], Benedikt Eggert[2], William Griggs[3], Shadab Anwar[1], Rantej Bali[1], Thomas Thomson[3], Eric Hirschmann[1], Ahmed G. Attallah[1], Heiko Wende[2], and Andreas Wagner[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]University of Duisburg-Essen, Duisburg, Germany — [3]The University of Manchester, Manchester, United Kingdom

Open volume defects in Fe60Al40 and Fe50Rh50 alloy thin films have been investigated with positron annihilation spectroscopy techniques. The distribution of open-volume defect types in Fe60Al40 thin films, i.e., mono-vacancies, triple defects as well as vacancy clusters has been estimated using positron annihilation lifetime spectroscopy. We show that the temperature driven re-ordering kinetics can be strongly modified by controlling the defect distribution through annealing and ion irradiation treatments. In particular, the splitting of vacancy clusters and triple defects into mono-vacancies by irradiation accelerates thermal diffusion, lowering the temperature necessary for re-ordering [J. Ehrler, et al., Acta Mater. 176 (2019) 167]. In case of B2 Fe50Rh50 thin films, ion irradiation induces a ferromagnetic behaviour in the initially antiferromagnetic thin films. The variation of open-volume defects during this transition has been tracked. We will demonstrate that irradiation induces open volume defects, whose concentration scales with ion fluence, providing insights on the types of defects associated with ferromagnetism in the Fe50Rh50 system.

MA 62.3 Fri 10:00 HSZ 401

Large Hall angle of the disordered B2 $Fe_{60}Al_{40}$ alloy — •Václav Drchal[1], Josef Kudrnovský[1], František Máca[1], Ilja Turek[2], and Sergii Khmelevskyi[3] — [1]Inst. of Physics, Czech Acad. Sci., Praha, Czech Republic — [2]Inst. of Physics of Materials, Czech Acad. Sci., Brno, Czech Republic — [3]Center for Computational Materials Science, Vienna University of Technology, Austria

The electronic and transport properties of the ordered B2 $Fe_{60}Al_{40}$ alloy which undergoes a continuous transition into disordered A2 $Fe_{60}Al_{40}$ phase are studied from first principles. Variation of the alloy disorder due to Fe antisites on Al sublattice is characterized by the partial long-range order. This is the simplest model of gradual disordering of the ordered phase due to the ion irradiation. The physical properties are strongly influenced by varying local environment of Fe atoms on both sublattices. This leads to the transition between a very low moment in the ordered phase to a high moment at large disorder. Similar behavior is found also for anomalous Hall conductivity and anomalous Hall angle. The disordered phase has a large Hall angle as contrasted with a negligible Hall angle for well ordered samples, which is in agreement with recent experiment.

MA 62.4 Fri 10:15 HSZ 401

Local structure after ion irradiation in FeRh thin films — •Johanna Lill[1], Benedikt Eggert[1], Katharina Ollefs[1], Sakura Pascarelli[2], Alexander Schmeink[3,4], Kay Potzger[3], Jürgen Lindner[3], Jürgen Fassbender[3,4], Thomas Thomson[5], Rantej Bali[3], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]ESRF, Grenoble, France — [3]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [4]Dresden University of Technology, Germany — [5]The University of Manchester, United Kingdom

B2 FeRh shows antiferromagnetic ordering in the thermodynamic stable phase, while the disordered structure exhibits a ferromagnetic and paramagnetic ordering. The disordered structure can be induced by ion irradiation [1]. In this work we investigate FeRh thin films for different irradiation fluences of 110 keV Ne^{+} by Fe K edge Extended X-ray absorption fine structure spectrosopy at low temperatures. For low irradiation fluences, we see an increase of the lattice parameter and an increase of static disorder by analysis of the mean square relative displacement. For higher fluences a change from the bcc to the fcc phase occurs. In addition, XRD measurements show similar behaviour to the EXAFS findings. From magnetometry, we determine an increase of the magnetisation and a shift of the phase transition to lower temperatures with rising irradiation fluence. Financial support by DFG (WE 2623/14-1) is acknowledged.

[1] A. Heidarian et al. J. Nucl Inst. Meth. B 358, 251 (2015)

MA 62.5 Fri 10:30 HSZ 401

Spin wave spectra of disordered materials — •Sebastian Paischer[1], Pawel Buczek[2], and Arthur Ernst[1] — [1]Johannes Kepler Universität Linz — [2]Hochschule für Angewandte Wissenschaften Hamburg

We use a new approach to calculate the Magnon dispersion of randomly disordered alloys based on the coherent potential approximation. The main features of our theory are the inclusion of both diagonal and off-diagonal disorder and the fact that we are not restricted to simple lattices and interactions. Additionally we are able to satisfy the Goldstone-theorem which is not always the case for many studies found in the literature. We augment the method to account for temperature dependence within the random phase approximation. In this talk I will present our results, e.g. the temperature- and concentration-dependence of disordered iron-cobalt alloys and the Heusler-alloy Ni_2MnSn of which we investigate the influence of antisite defects.

MA 62.6 Fri 10:45 HSZ 401

Impact of correlation effects on the magneto-optical Kerr effect in transition metals and their alloys — •Andreas Held[1], Ján Minár[2], and Hubert Ebert[1] — [1]Department Chemie, Ludwig-Maximilians-Universität München — [2]New Technologies-Research Center, University of West Bohemia, Pilsen

The magneto-optical Kerr effect (MOKE) is a well-established tool for investigating the properties of magnetic systems. Originating from the subtle interplay between magnetic order and spin-orbit coupling, a proper theoretical description of MOKE requires an appropriate framework. Such a scheme has been worked out by Huhne [1] on the basis of the fully relativistic spin-polarized Korringa-Kohn-Rostoker method [2]. To allow for the treatment of substitutionally disordered systems, the approach has been combined with the coherent potential approximation (CPA) alloy theory. The extended scheme gives access to the configurationally averaged optical conductivity tensor and this way to the corresponding complex Kerr angle. The additional combination with Dynamical Mean Field Theory (DMFT) [3] allows in particular to investigate the influence of correlation effects on the MOKE in disordered systems. Corresponding results for pure Ni, Fe and Co as well as disordered Fe_xCo_{1-x} and Co_xPt_{1-x} alloys are presented and compared with experimental data.

[1] Huhne, Ebert, *Phys. Rev. B* **60**, 12982 (1999); Huhne, Ebert, *Phys. Stat. Sol. B* **215**, 839 (1999)

[2] Ebert, Ködderitzsch, Minár, *Rep. Prog. Phys.* **74**, 096501 (2011)

[3] Minár et al., *Phys. Rev. B* **72**, 045125 (2005)

MA 62.7 Fri 11:00 HSZ 401

Local short-scale correlations and the origin of pseudo-diamagnetism — •Malvika Tripathi[1], T. Chatterji[2], H. E. Fischer[2], R. J. Choudhary[1], and D. M. Phase[1] — [1]UGC-DAE Consortium for Scientific Research,Indore-452001, India — [2]Institut Laue-Langevin, 38042 GRENOBLE Cedex, France

Here we describe why the antiferromagnetically ordered $GdCrO_3$ behave in a diamagnetic way under certain conditions, by monitoring the evolution of the microscopic global and local magnetic phases. High energy neutron diffraction reveals that magnetic ordering comprises three distinct magnetic phases at different temperatures: G_x^{Cr},A_y^{Cr},F_z^{Cr} below Néel temperature = 171 K; (F_x^{Cr}, C_y^{Cr}, G_z^{Cr})•($F_x{}^{Gd}$,$C_y{}^{Gd}$) below 7 K and an intermediate phase for 7 K $\leq T \leq$ 20 K in the vicinity of spin-reorientation phase transition. Although, bulk magnetometry reveals a huge negative magnetization (NM) in the terms of both magnitude and temperature range; the long-range magnetic structure and derived ordered moments remain silent about any signature of NM. Real-space analysis of the total scattering suggests significant magnetic correlations extending up to $\sim$ 9 Å. Accounting for these short-range correlations with a spin model reveals spin frustration in the S= 3 ground state, comprising competing first, second and third next nearest exchange interactions with values J_1 = 2.3 K, J_2 = -1.66 K and J_3 = 2.19 K in presence of internal field, governs the observance of NM in $GdCrO_3$.

MA 62.8 Fri 11:15 HSZ 401

Uniform Heisenberg spin chain in sarrabusite $Pb_5Cu(SeO_3)_4Cl_4$ — •Ekaterina Kozlyakova, Artem Moskin, Alisher Murtazoev, Peter Berdonosov, and Alexander Vasiliev — Lomonosov MSU, Moscow, Russia

One-dimensional antiferromagnets have exotic disordered ground states. The uniform half-integer spin chain does not present a gap in the triplet excitation spectrum and it is disordered in an isotropic Heisenberg case. In any real material an ideal S = 1/2 chain cannot exist because an infinitesimal interchain coupling would give rise to long-range magnetic order at finite temperatures. [1, 2] In this work we present novel uniform spin chain compound $Pb_5Cu(SeO_3)_4Cl_4$ that demonstrates no long-range magnetic ordering up to 2 K. Its magnetic susceptibility agrees well with the Bonner-Fisher's model with J = 129K for Heisenberg AFM S = 1/2 spin chain [3]. Thus, $Pb_5Cu(SeO_3)_4Cl_4$ is one of the very few uniform spin chains where no long-range magnetic ordering or any singlet formation were observed above 2 K, while J is of the order of 100 K.

[1] E. Lieb, et al. Annals Phys. 16, 407-466 (1961).
[2] D.C. Johnston, et al. Phys. Rev. B 61, 9558-9606 (2000).
[3] J.C. Bonner & M.E. Fisher. Phys. Rev. A 135, 640-658 (1964).