MA 9: Magnetic Materials I

Time: Monday 14:45–17:00 Location: HSZ 401

MA 9.1 Mon 14:45 HSZ 401

Magnetoresistance and Anomalous Hall Effect of Ferromagnetic Half-Metallic Heusler Compound Co_2FeSi — •Dirk Bombor, Oleg Volkonskyi, Christian G. F. Blum, Steven Rodan, Mahmoud Abdel-Hafiez, Anja Wolter, Sabine Wurmehl, Christian Hess, and Bernd Büchner — Leibnitz Institute for Solid State and Materials Research, IFW Dresden, Germany

Electronic transport properties of the Heusler Compound Co_2FeSi have been studied. This compound is a soft ferromagnet which is predicted to be half-metallic — this means complete spin polarization of the conducting electrons. Its resistivity behaviour in dependence of the temperature is typical for ferromagnetic compounds, and is dominated by scattering of the charge carriers at spin fluctuations. This scattering is suppressed at low temperatures due to an energy gap where this gap can be attributed to the half-metallic property of this compound. A positive magnetoresistance at low temperatures and a negative magnetoresistance at high temperatures has been observed as well as an anomalous Hall effect which is found to be driven by scattering of conducting electrons at magnetic scattering centres.

MA 9.2 Mon 15:00 HSZ 401

Magnetism of quaternary Heusler alloys — •Josef Kudrnovsky[1], Shyamal Bose[2], Ilja Turek[3], and Vaclav Drchal[1] — [1]Institute of Physics AS CR, Prague — [2]Brock University, St. Catharines — [3]Institute of Physics of Materials AS CR, Brno

The electronic properties, exchange interactions, finite-temperature magnetism and transport properties of random Ni2MnSn quaternary Heusler alloys doped with Cu- and Pd-atoms are studied theoretically by means of first-principles calculations over the entire concentration range. While the magnetic moments are only weakly dependent on the alloy composition, the Curie temperatures exhibit strongly non-linear behavior with respect to Cu-doping in contrast with an almost linear concentration dependence in the case of Pd-doping. The residual resitivity obey the Nordheim rule while the dominating contribution to the temperature-dependent resistivity is due to thermodynamical fluctuations originating from the spin-disorder, which, according to our calculations, can be described reasonably well via the disordered local moments model. The present parameter-free theory agrees qualitatively and also reasonably well quantitatively with all available experiments.

MA 9.3 Mon 15:15 HSZ 401

Structural, magnetic and electronic properties of a new silicide MnPtSi — •Monika Gamza[1,2], Sarah Ackerbauer[1], Andreas Leithe-Jasper[1], Walter Schnelle[1], Helge Rosner[1], and Yuri Grin[1] — [1]MPI CPfS Dresden — [2]Institute of Materials Science, University of Silesia, Katowice, Poland

Recent results concerning giant exchange-derived magnetoelastic coupling in a metamagnet MnCoSi (TiNiSi-type structure) [1] as well as intriguing magnetic properties of the isostructural compounds MnTX (T = transition metal element; X = Si, Ge) [2] prompted us to search for consecutive members of this family.

Here, we report on the crystal structure, electronic structure and magnetic properties of the new compound MnPtSi. The Mn K XAS data indicate a divalent state of Mn ions. The effective moment derived from high-temperature magnetic susceptibility of $4.1\mu_B$ indicates an intermediate spin state of Mn ions. These findings have been confirmed by first principles electronic structure calculations. Thermodynamic measurements revealed two successive magnetic phase transitions at $T_C \approx 350$ K and $T_N \approx 326$ K. The FM to AFM transition is accompanied by a large magneto-volume effect ($\Delta V/V$ reaches $\sim$1.4%) and a change in Mn-Mn distances of up to 1%. The origin of the strongly anisotropic thermal expansion is analyzed.

[1] Barcza A. *et al.*, Phys. Rev. Lett. (2010) **104** 247202

[2] Eriksson T. *et al.*, Phys. Rev. B (2005) **71** 174420 and references there in

MA 9.4 Mon 15:30 HSZ 401

Ab initio modeling of Fe-Mn based alloys — •Denis Comtesse, Heike C. Herper, Mario Siewert, Alfred Hucht, and Peter Entel — Faculty of Physics - University of Duisburg-Essen, 47048 Duisburg, Germany

We present ab initio calculations of structural and magnetic properties of iron-manganese alloys over a wide range of compositions using VASP [1]. We add different amounts of carbon and silicon on complete relaxed interstitial and substitutional lattice positions and analyze the changes of the magnetic exchange interactions J_{ij}. The exchange parameters are used for Monte Carlo simulations of the Heisenberg model to extend the analysis of the magnetic behavior to finite temperatures and to determine the magnetic transition temperatures. In order to examine the influence of disorder we employed the KKR-CPA method [2] and calculated the exchange parameters for various types of disorder. We find a strong dependence of the critical temperature on the disorder and the carbon content. The disorder always tends to reduce the transition temperature. In case of high carbon concentrations, ordered systems show a strong relation between the iron-manganese composition and the transition temperature.

[1] G. Kresse and J. Furthmüller, Phys. Rev B **54**, 11169 (1996)

[2] The Munich SPR-KKR package, version 3.6, H. Ebert et al.

MA 9.5 Mon 15:45 HSZ 401

The effect of boron doping on the magnetostriction of Fe-Ga and Fe-Al samples — •Mathias Doerr[1], Claudio Teodoro dos Santos[2], Sergey Granovsky[1], Cristina Bormio-Nunes[2], and Michael Loewenhaupt[1] — [1]TU Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany. — [2]Universidade de Sao Paulo, Escola de Engenharia de Lorena, CA 116 CEP 12602-810 Lorena, Brazil.

Fe-Ga (Galfenol) based alloys are used in a number of magnetomechanical applications because of the high magnetostriction values of more than 100 ppm at room temperature. The addition of boron inhibits the crystallographic ordering of the alloys and stabilizes the disordered A2 structure that is responsible for the high striction values. Especially, polycrystalline and rapid cooled Fe-Ga-B and Fe-Al-B samples were investigated in our project. Magnetization and longitudinal as well as transversal magnetostriction measurements at temperatures of 5K, 80K and 300K show a similar effect of the amount of B as found on single crystals. Whereas the saturation magnetization is nearly the same and mainly determined by the Fe content, a dependence of the striction values on the amount of B is visible (more than 10% in the Fe-Al system). The results illustrate the influence of the stoichiometry and the preparation conditions on the magnetomechanical properties.

MA 9.6 Mon 16:00 HSZ 401

Development of magnetic moments in $Fe_{1-x}Ni_x$ - alloys — Benjamin Glaubitz, Stefan Buschhorn, Frank Brüssing, and •Hartmut Zabel — Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum

$Fe_{1-x}Ni_x$ alloys have been studied intensively in the past because of their unique properties, such as the soft magnetic properties at x = 0.8 and the martensitic bcc-fcc transition at x = 0.35. The total magnetic moment as a function of alloy concentration follows by and large the Slater Pauling curve, but not in the region of the martensitic transition, where a strong drop is observed, which has been taken as a sign for strong magneto-volume fluctuations, also known as the invar effect. Using XMCD methods, we have analyzed the individual magnetic moments of Fe and Ni across the alloy concentration range, including their spin and orbital contributions, and we have compared those with the average moments determined by VSM measurements. We find a very good agreement between both methods, with the individual moments showing some fluctuations at the invar concentration but no anomaly. We will discuss the results in the light of recent theoretical predictions [1].

[1] I.A. Abrikosov, A.E. Kissavos, F. Liot, B. Alling, S.I. Simak, O. Peil, A.V. Ruban, Phys. Rev. B **76**, 014434 (2007)

MA 9.7 Mon 16:15 HSZ 401

Precursor Phenomena at the Magnetic Ordering of the cubic Helimagnet FeGe — •Michael Baenitz[1], Heribert Wilhelm[2], Marcus Schmidt[1], Ulrich K. Rössler[3], Alexei N. Bogdanov[3], and Andrey A. Leonov[3] — [1]MPI CPfS, Noethnitzer Str. 40, 01187 Dresden — [2]Diamond Light Source Ltd., Chilton, Didcot, OX11 0DE,

United Kingdom — [3]IFW Dresden, Postfach 270116, 01171 Dresden

We report on detailed magnetic measurements on the cubic helimagnet FeGe in external magnetic fields parallel to the [100] direction and temperatures in the vicinity of the onset of long-range magnetic order at $T_c \approx 278$ K. Depending on the temperature and field, a helical state ($H < H_{c1}$), a conical phase ($H_{c1} < H < H_{c2}$), or the so-called A-phase were observed below H_{c2} at which the field-polarized state occurs. Precursor phenomena found above T_c display a complex succession of temperature-driven cross-overs and phase transitions. The A-phase pocket is split in at least two distinct areas, A_1 and A_2. The area A_1 at lower fields shows clear lines of transitions into the conical phase at lower temperature and into the A_2 area at higher fields. The area A_2 appears to transform continuously into the conical phase. Relying on a modified phenomenology for chiral magnets, the A_1 phase could indicate existence of a $+\pi$ Skyrmion lattice, however, the A_2 phase seems related to helicoids propagating in directions perpendicular to the applied field. We suggest that the observation of this A_2-phase can be explained by hexagonal arrays of spiral domains consisting essentially of helicoids.

MA 9.8 Mon 16:30 HSZ 401

Evaluation of magnetic anisotropy energy in a relativistic picture — •Toshio Miyamachi[1], Tobias Schuh[1], Shih-Yu Wu[2], Chein-Cheing Kuo[2], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Germany — [2]Department of Physics, National Sun Yat-sen University, Taiwan

The magnetic stability of nanostructures is relied on the magnetic anisotropy energy (MAE). The MAEs of small clusters are experimentally evaluated with two different models. Firstly, the effective spin model is used for inelastic tunneling spectroscopy (ITS) [1]. In this model, only an effective spin S is treated. Secondly, the Bruno model is used for X-ray magnetic circular dichroism (XMCD), where the MAE is linked to an anisotropy of the orbital momentum L [2]. To bring these models together, we propose a relativistic model with the total angular momentum J = L + S. Within our relativistic model, the MAE of a Co single atom on Pt(111) obtained with ITS [3] is reevaluated as 13.7 meV/atom. The validity of our model is verified by comparing calculated magnetization curves with experimental ones obtained by XMCD and spin-polarized scanning tunneling microscopy [4,5].

[1] C. F. Hirjibehedin et al., Science 317, 1199 (2007)
[2] P. Pruno, Phys. Rev. B 39, 865 (1989)
[3] T. Balashov et al., Phys. Rev. Lett. 102, 257203 (2009)
[4] P. Gambardella et al., Science 300, 1130 (2003)
[5] F. Meier et al., Science 320, 82 (2008)

15 min. break