MA 21: Magnetic Materials

Time: Wednesday 15:15–18:00 Location: H23

MA 21.1 Wed 15:15 H23

Phase Stability in Magnetocaloric La(Fe,Si)$_{13}$ Ribbons — •Maria Krautz, Jian Liu, Julia Lyubina, Konstantin Skokov, Ludwig Schultz, and Oliver Gutfleisch — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden

In the last decade several materials, exhibiting a giant magnetocaloric effect (MCE), have been studied. Magnetic refrigeration appears now as a viable alternative to conventional gas compression/expansion techniques. Some alloys with the $NaZn_{13}$-structure are of high interest, as they show a first-order phase transition in the vicinity of the Curie temperature, leading to a giant MCE. As the binary $LaFe_{13}$-phase does not exist, it has to be stabilised by adding a third element such as Al or Si. In order to remove the primary α-Fe and obtain nearly pure 1:13-phase from the as-cast alloy, a prolonged heat treatment taking up to several weeks is usually performed. The melt-spinning technique is proven to be very useful to synthesize various functional magnetic materials with a homogenous chemical composition and a refined microstructure. Here we applied this technique to the La-Fe-Si system. After a short time annealing of only a few hours, the 1:13-phase is established in the melt-spun ribbons. However, little knowledge about the pseudobinary phase diagram of La(Fe,Si)$_{13}$ is available so far. Therefore, melt-spun alloys with different Si contents were annealed at different temperatures. The structure was studied by XRD (Rietveld-refinement) and SEM and correlated with magnetic data. In view of application, the significant volume change of the 1:13-phase during the magnetic phase transition is analysed.

MA 21.2 Wed 15:30 H23

Investigations of highly ordered, half-metallic Co_2FeSi single crystals — •C. G. F. Blum[1,2], S. Wurmehl[1], G. Behr[1], C. Hess[1], B. Büchner[1], J. Barth[2], C. A. Jenkins[2], C. Felser[2], S. Riegg[3], A. Reller[3], and J. T. Kohlhepp[4] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Helmholtzstraße 20, D-01069 Dresden — [2]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg-University, Mainz — [3]Universität Augsburg, D-86159 Augsburg — [4]Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

In this presentation the properties of highly ordered, halfmetallic Co_2FeSi single crystals will be shown. A wide variety of properties, such as half-metallicity and semiconductivity, is found among the Heusler compounds. In order to separate intrinsic and extrinsic properties, high quality single crystals are required. Here we report on crystals of the half-metallic ferromagnet Co_2FeSi [1], grown with different techniques. All crystals show excellent ordering, probed by XRD and NMR, resulting in outstanding electrical behavior. Low residual resistivity and high residual-resistivity-ratio is found. All Co_2FeSi crystals show a plateau in resistivity below 50 K, which might point to half-metallic ferromagnetism. The cross-over from this unusual to more conventional transport (T^2 dependence) around 50 K indicates the onset of spin flip scattering and thus is indispensable for understanding the strong temperature dependence of Co_2FeSi tunneling magnetoresistance-devices. The authors gratefully acknowledge financial support by the DFG (Research Unit 559). [1] Blum et al. Appl. Phys. Lett. 95 161903 (2009).

MA 21.3 Wed 15:45 H23

Disorder Effects on the Magneto-Crystalline Anisotropy Energy of Strained Fe-Co Alloys — •Carsten Neise, Stephan Schönecker, Manuel Richter, Klaus Koepernik, and Helmut Eschrig — IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

Tetragonally distorted $Fe_{1-x}Co_x$ alloys recently attracted interest due to their potential applicability as new media for high density recording, combining a large uniaxial **M**agneto-**C**rystalline **A**nisotropy with a large saturation magnetisation for certain chemical compositions x and certain tetragonal distortions. Previous calculations by Burkert *et. al.* [Phys. Rev. Lett. 93, 027203 (2004)] disregarded volume relaxation, which is present in epitaxially grown layers and may alter the magnetic properties of these alloys. We investigated this and the influence of disorder on the MCA and on the magnetic moment of $Fe_{1-x}Co_x$ alloys along the epitaxial Bain path. Two different methods were used to describe disorder, (i) the virtual crystal approximation, and (ii) a stochastic average of supercells with randomly distributed atoms. Comparison with the ordered structures of the $L1_0$ and the $L1_2$ phases reveals the impact of disorder on the magnetic properties. We employed the **f**ull **p**otential **l**ocal **o**rbital program package FPLO [*http://www.fplo.de*] for our density functional calculations.

MA 21.4 Wed 16:00 H23

Interplay between chemical and magnetic orders in alloys — •Josef Kudrnovsky[1], Vaclav Drchal[1], and Ilja Turek[2] — [1]Institute of Physics AS CR, Prague — [2]Institute of Physics of Materials AS CR, Brno

Based on the first-principles modeling we will investigate the interplay between the chemical and magnetic orders in the magnetic transition metal alloys. As a case study we will investigate the change of magnetic order due to the chemical order-disorder transformation in fcc-Ni(75)Fe(25), fcc-Ni(75)Mn(25), and bcc-Fe(50)Al(50). The theoretical modeling is done in two steps: in the first-step we will determine the electronic structure of studied magnetic alloys in both disordered and ordered state (Cu3Au-structure for fcc NiFe and NiMn alloys, CsCl-structure for bcc FeAl alloys) by using the tight-binding linear muffin-tin orbital method suitable for description of transition-metal alloys. The chemical disorder is treated in the framework of the coherent-potential approximation. In the second step, the calculated electronic structure is used to estimate the pair exchange interactions by using the method of infinitesimal rotations (the construction of the classical Heisenberg model) for ordered and disordered phases. We will demonstrate that chemical ordering strongly influences the magnetic order in fcc-NiMn and bcc-FeAl alloys. This can be understood on the basis of calculated exchange Heisenberg parameters of alloys in both ordered and disordered phases.

MA 21.5 Wed 16:15 H23

Magneto-impedance measurements on iron whiskers — •Matthäus Langosch, Haibin Gao, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, D-66123 Saarbruecken, Germany

After the discovery of the giant magneto-impedance (GMI) effect in 1994, the research on GMI mainly focuses on the enhancement of the effect by developing new materials and on potential applications. But a better understanding of the effect itself is as well needed. GMI measurements on iron single crystals (iron whiskers) with <100> growth direction were carried out at room temperature. The GMI effect of the whiskers has been observed as a function of driving current and frequency. A maximum MI value of 63% was found for the chosen samples having a particularly simple domain structure. MOKE imaging was employed to investigate more clearly the relationship between GMI effect and the respective domain structures. It was found that the magnetic-field-dependent skin effect provides major contributions.

MA 21.6 Wed 16:30 H23

Magnetic detector based on giant magnetoimpedance and its application to vehicle detection — Qing Zhang[1], •Haibin Gao[2], Zhenjie Zhao[1], and Uwe Hartmann[2] — [1]Department of Physics, East China Normal University, 3663 Zhongshan North Road, 200062 Shanghai, P.R. China — [2]Institute of Experimental Physics, Saarland University, D-66123 Saarbruecken, Germany

A field detector based on the giant magnetoimpedance (GMI) effect is developed. The GMI sensor is made of a $Co_{68.15}Fe_{4.35}Si_{12.5}B_{15}$ microwire with a diameter of $25\mu m$ and a length of $5mm$. A pick-up coil is around the microwire. The driving ac current through the wire induces an axial magnetization variation and thus a voltage in the pick-up coil. The field dependence of the second harmonics of this voltage is measured. The characteristics of the complete detector in terms of sensitivity, resolution, linearity, and temperature behavior were obtained under laboratory conditions. A $10pT$ magnetic field at a frequency of 40 Hz was detected. The output signal change is lower than 4 x $10^{-4}/K$ in the working range of -40^0C to 85^0C. A first field test result on vehicle detection will be presented.

15 min. break

MA 21.7 Wed 17:00 H23

Effect of non-magnetic impurities on the ferromagnetism of Mn_5Ge_3 — •Ivetta Slipukhina[1,2], Emmanuel Arras[1], Phivos Mavropoulos[2], and Pascal Pochet[1] — [1]Laboratoire de simulation atomistique, SP2M, INAC, CEA, 38054 Grenoble cedex 9, France — [2]Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

Mn_5Ge_3 is a ferromagnet with a magnetisation of 2.6 μ_B/Mn, spin polarisation $P_0 = 42\%$ and T_C=304 K. Experimentally, interstitial C in this material enhances its ferromagnetic properties and results in essentially increased T_C. To understand the nature of exchange interactions in doped Mn_5Ge_3 and their dependence on the chemistry and concentration of interstitials, we performed first principles electronic structure calculations, utilizing the Korringa-Kohn-Rostoker Green function method within the Coherent-Potential Approximation [1]. The transition temperatures are calculated by means of Monte Carlo method, using a classical Heisenberg Hamiltonian and calculated exchange constants. A non-monotonous variation of the T_C with x is found in $Mn_5Ge_3C_x$, reflecting the non-monotonous change of the impurity mediated exchange interactions [2]. Strong enhancement of T_C is predicted for B- and N-doped Mn_5Ge_3 [3], making them, along with the $Mn_5Ge_3C_x$, promising candidates for spintronics applications.

[1] H. Ebert and R. Zeller, The SPR-TB-KKR package, http://olymp.cup.uni-muenchen.de/ak/ebert/SPR-TB-KKR.
[2] I. Slipukhina *et al.*, Appl. Phys. Lett. **94**, 192505 (2009).
[3] I. Slipukhina, E. Arras, and P. Pochet, in preparation.

MA 21.8 Wed 17:15 H23

Magnetic measurements on Tb_5Ge_3 — •Ariane Haase[1,2], Mathias Doerr[2], Marek Bartkowiak[1], Ramzy Daou[1,3], Yurii Skourski[1], Martin Rotter[4], and Marc Uhlarz[1] — [1]Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf, 01314 Dresden — [2]Institut für Festkörperphysik, TU Dresden, 01069 Dresden — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden — [4]University of Oxford, Department of Physics, Oxford OX1 3PU

Tb_5Ge_3 is a weak antiferromagnet, which orders at 83 K. It crystallizes in Mn_5Si_3-type hexagonal structure with two different positions for the Tb^{3+} ions. The hexagonal ab-plane is the easy plane of magnetization.

Magnetization and magnetostriction measurements have been done on a single crystal in static fields up to 30 T and in pulsed fields up to 50 T. In addition to the antiferromagnetic phase, three more phases were found in fields in the ab-plane at low temperatures. Surprisingly, the measurements along the b-axis do not resemble the a-axis properties which indicates an anisotropy in the hexagonal plane. Initial model calculations reveal the anisotropy of the magnetic exchange, which is dominant over the crystal electric field effect, as cause. The hard c-axis shows only one phase transition at 5 T followed by a nearly linear magnetization and magnetostriction slope which is attributed to a steady-going rotation of the moment.

MA 21.9 Wed 17:30 H23

Grain refinement in HDDR $Nd_2Fe_{14}B$ powders by high pressure reactive milling — •Konrad Güth, Julia Lyubina, Ludwig Schultz, and Oliver Gutfleisch — IFW Dresden, Institut für Metallische Werkstoffe, Postfach 270016, D-01171 Dresden, Germany

The HDDR process (Hydrogenation Disproportionation, Desorption, Recombination) is a unique method to produce highly coercive powders for resin bonded permanent magnets. The process is carried out under carefully controlled hydrogen atmosphere resulting in $Nd_2Fe_{14}B$ crystallites with a size of about 300 nm well-oriented within micrometer-sized particles. A further increase of the energy product in these HDDR powders may be achieved via inter-grain exchange coupling that requires the decrease of the grain size by one order of magnitude. A novel approach is the high pressure reactive milling (HPRM) technique prior to the hydrogen desorption and recombination process. The NdFeBGaNb starting alloy is milled in dedicated ball vial under 50 bar hydrogen pressure for 5 hours. After recombination at elevated temperatures under reduced hydrogen atmosphere the final powder shows a much smaller grain size than that in the HDDR processed powder. Phase analysis and grain size determination were performed using Rietveld refinement of x-ray data. High resolution scanning electron microscopy (HR SEM LEO 1530 GEMINI) was used to study the microstructure. In order to investigate the texture of the final magnet, the powder is aligned applying a transverse magnetic field of 2 T during pressing. The influence of the HPRM on the structure and magnetic properties of the HDDR Nd-Fe-B alloys will be discussed.

MA 21.10 Wed 17:45 H23

Magnetic properties of the main group diradical ion 5,5'-Bis(1,2,3,4-trithiazolium) in a solid state matrix — •Manuel Presnitz[1], Ernst-Wilhelm Scheidt[1], Wolfgang Scherer[1], and Jack Passmore[2] — [1]Lehrstuhl für Chemische Physik und Materialwissenschaften, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — [2]Department of Chemistry, University of New Brunswick, Fredericton NB E3B 6E2, Canada

The diradical nature of the main group molecule $(CNSSS)_2$, systematic name 5,5'-Bis(1,2,3,4-trithiazolium), is remarkable because it is – like the prominent diradical O_2 – a non sterically hindered main group compound, which retains its paramagnetic characteristics also in the solid state. Here the $(CNSSS)_2$ diradical ions are embedded in a PnF_6 (Pn = As, Sb) matrix.

The specific heat $C(T)$ and magnetic susceptibility $\chi(T)$ data (for SbF_6 matrix) show some irreversible behavior during the first cooling stage down to 2 K. By subsequent heating/cooling cycles different states seem to be accessible until a final reversible behavior (χ_{rev}) is observed.

The magnetic susceptibility of different model systems was fitted to χ_{rev} but the distinction between an alternating spin chain (Johnston *et al.*) and spin ladder (Barnes/Riera) is not possible based on experimental results for $\chi(T)$ only. Hence, to gain deeper insight into the magnetic coupling mechanism, our $\chi(T)$ measurements are complemented by *ab initio* calculations to obtain *inter*- and *intra*-molecular coupling constants and disqualify one of the models.