MA 50: Soft and hard permanent magnets

Time: Thursday 15:00–16:45 Location: EB 301

MA 50.1 Thu 15:00 EB 301

Improving magnetic properties of Ce-Fe permanent magnets with La doping — •Martin Hoffmann[1,2], Munehisa Matsumoto[2], Takashi Miyake[3], and Hisazumi Akai[2] — [1]Institute for Theoretical Physics, Johannes Kepler University Linz, Austria — [2]Institute for Solid State Physics, University of Tokyo, Japan — [3]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

Powerful permanent magnets are a crucial component in electric motors and gen- erators, while the most powerful magnets available nowadays are alloys of rare-earth (RE) elements and magnetic transition metal elements. Unfortunately, the availability of the RE elements of the best magnets is strongly limited. Therefore, different paths are undertaken in order to find better or cheaper permanent magnets. We study theoretically the effect of La and Co doping on the magnetic properties of potentially cheaper Ce-Fe permanent magnets with 1-2, 1-5, or 1-12 composition.

We studied the magnetic moments, coupling, anisotropy and the Curie temperature. These quantities and their dependence on the doping have to be at first better understood and in a second step optimized for a good performance of the magnets. We found significant changes in the calculated magnetic properties when mixing Ce with La and Fe with Co. Looking at the formation energy of the compounds identifies possible stable concentration regimes where new compounds could be synthesized.

MA 50.2 Thu 15:15 EB 301

Hard magnetic Fe-Hf-Sb based intermetallic compound of hexagonal Laves phase structure — •Dagmar Goll, Thomas Gross, Ralf Loeffler, Ulrich Pflanz, Tim Vogel, Andreas Kopp, Tvrtko Grubesa, and Gerhard Schneider — Aalen University, Materials Research Institute (IMFAA), Aalen, Germany

Rare earth free phases are searched for possible candidates for novel hard magnets to realize efficient energy converters. By experimental bulk high-throughput screening the ternary system Fe-Hf-Sb, off-stoichiometric $(Fe,Sb)_{2+x}Hf_{1-x}$ with a composition of Fe60.0-Hf26.5Sb13.5 with potential as hard magnetic phase has been discovered. By quantitative domain structure analysis, interesting intrinsic magnetic properties of $J_s \approx 1$ T and $K_1 \approx 1.5$ MJ/m^3 are estimated at room temperature. By magnetometry, bulk intrinisic properties of $J_s \approx 0.7$ T and $K_1 \approx 1.4$ MJ/m^3 are found from the approach to ferromagnetic saturation. X-ray diffraction analysis proves the presence of hexagonal C14 Laves phase structure. Alloying elements like Co or Mn can modify the crystal structure and ferromagnetic behavior. In addition, rapid quenching is applied to realize nanocrystalline magnetic materials thereof. The project is supported by Ministry of Economic Affairs, Labor and Housing Baden-Wuerttemberg.

MA 50.3 Thu 15:30 EB 301

$Li[Li_{1-x}Co_x]AE_2N_2$ (AE = Ca, Sr): New examples for magnetically anisotropic transition metals in linear coordination — •Tanita J. Ballé[1], Peter Höhn[2], and Anton Jesche[1] — [1]EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany — [2]Max-Plack-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

$Li_2[Li_{1-x}Fe_x]N$ is one of the scarce rare-earth free hard magnets and shows a huge magnetic anisotropy and the highest known coercivity field of more than 11 T! These properties are attributed to the unquenched orbital moment of iron, enabled by the perfect linear, twofold coordination of iron between nitrogen [1]. In order to investigate the necessity as well as sufficiency of this geometrical motive, we studied similar compounds [2]. We will show that large coercivity fields are not restricted to iron. Isothermal and temperature dependent magnetic measurements were performed on $Li[Li_{1-x}Co_x]AE_2N_2$, which contains cobalt in linear coordination. Ferromagentic ground states with a coercivity of ~ 0.5 T are observed at 2 K. The Hysteresis vanishes at 76 K for AE = Ca and 43 K for AE = Sr, respectively, and is clearly reflected in the temperature dependence of the magnetization. We conclude that the structural motive of a transition metal in linear coordination with only two neighbours, allows to predict materials with stable magnetic properties. [1] A. Jesche *et al.* Nat. Commun. **5**:3333. doi: 10.1038/ncomms4333 (2014) [2] P. Höhn, TJB *et al.* Inorganics 4, **42** (2016)

MA 50.4 Thu 15:45 EB 301

Magnetic properties of iron based 1:12 permanent magnets from first principles — •Olga Yu. Vekilova, Olle Eriksson, and Heike C. Herper — Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

The iron-rich compounds are very promising for permanent magnet applications because of their large magnetic moments, rather high coercivity and sufficiently high Curie temperature. The 1:12 compounds with the $ThMn_{12}$-type structure are among the best candidates. However, light rare earths and iron cannot be stabilized in a binary 1:12 compound without a third dopant, like Ti or V. Such substitution results in a significant decrease in the saturation magnetization of the compound and can also influence magnetocrystalline anisotropy and Curie temperature. We addressed the problem from first principles. Starting from the known stable $NiFe_{11}Ti$ and $SmFe_{10}V_2$ phases we tried to improve the magnetic properties by reducing the content of Ti and V respectively. The phase stabilities of $NdFe_{11-x}Ti_x$ and $SmFe_{10-x}V_x$ were calculated and compared to the available experimental data. We further substituted Nd in $NdFe_{11-x}Ti_x$, partially by Y, which is a light 4d element, and revealed how the content of Nd and Ti can improve the magnetocrystalline anisotropy.

MA 50.5 Thu 16:00 EB 301

Noncollinear magnetism in Mn_3X (X=Sn, Ge, Ga) compounds — •Bendegúz Nyári, András Deák, and László Szunyogh — Budapest University of Technology and Economics, Budapest, Hungary

The intermetallic compounds Mn_3X (X=Sn, Ge, Ga) in hexagonal crystal structure show complex magnetic behaviour. Neutron diffraction [1] and theoretical [2] studies reveal that these compounds have a triangular spin configuration displaying weak ferromagnetic deformation. In a recent theoretical work [3] nonplanar spin-configurations were also reported. In this work we investigate theoretically the formation of non-collinear spin configurations. Spin-model parameters were obtained from a spin-cluster expansion (SCE) technique and by fitting rotational energies to analytic expressions derived from group-theoretical arguments. A model based on six magnetic sublattices confirms indeed a planar weak ferromagnetic ground state. In case of Mn_3Ge, the investigation of the static spin-susceptibilty, $\chi(\mathbf{q})$, indicates, however, that the system can be stabilized in a complicated magnetic structure at finite wavevector $\mathbf{q}$. By using tensorial spin-interactions obtained from SCE, Monte-Carlo simulations are performed to study such complex magnetic ground states.

[1] S. Tomiyoshi et al., J. Magn. Magn. Mater. 54–57, 1001 (1986)
[2] L. M. Sandratskii and J. Kübler, Phys. Rev. Lett. 76, 4963 (1996)
[3] J. Kübler and C. Felser, Europhysics Lett. 108, 67001 (2014)

MA 50.6 Thu 16:15 EB 301

Using FORC to understand the microstructure-micromagnetism relationship in supermagnets — •Sven Erik Ilse, Felix Gross, Joachim Gräfe, and Eberhard Goering — Max Planck Institute for Intelligent Systems, Germany

First-order-reversal-curve (FORC) diagrams yield a great variety of magnetic information such as coercive and interaction field distributions. We have recently demonstrated that FORC on MnBi can provide deep insight in the relationship between magnetism and microstructural properties, as grain size distributions and grain shapes[1]. Following these studies we investigated neodymium based permanent magnets and their FORC density relationship to microstructural properties. We systematically manipulated the microstructure of the samples by consecutive annealing (at different temperatures and intervals), and correlated their grain size-distributions with FORC diagrams. Our analysis of the grain size distributions showed that the grain sizes shift to higher diameters and the distribution broadens for longer annealing times. The room temperature FORC diagrams revealed that the width of the coercive field distribution increases. Correlating the widths of grain size- and coercive field- distributions reveals a linear dependence, which enables us to draw conclusions about grain sizes directly from FORC measurements. Our results demonstrate the versatility of FORC investigations providing rich additional information and enabling detailed understanding of coercive and interaction field distributions of our samples related to microstructure and grain size distributions.

[1] S. Muralidhar, et al., Physical Review B 95.2 (2017): 024413.

MA 50.7 Thu 16:30 EB 301

Anisotropic Effects of the Grain Boundary Diffusion Process (GBDP) in Textured Nd Fe B Magnets — •Tim Helbig, Andreas Abel, Simon Sawatzki, and Oliver Gutfleisch — TU Darmstadt

The Grain Boundary Diffusion Process (GBDP) is an industrially applied process to increase the coercivity of Nd-Fe-B sintered magnets using a minimal amount of heavy rare earth elements (HRE). In this process, the fully sintered and textured magnets are coated with a HRE or HRE compound and exposed to a heat treatment, causing the HRE to diffuse into the magnet. In order to investigate the texture dependence of this diffusion, a single face of a brick shaped sample was covered with Dy or Dy alloy and heat treated. Subsequently a coercivity profile was determined, by cutting the sample into small slices and measuring their coercivity individually. Simultaneously a second coercivity profile was derived by measuring the coercivity of the remaining sample piece after cutting each respective slice. The two data sets were compared allowing not only conclusions regarding the anisotropic grain boundary diffusion of Dy or Dy alloy, but also showed a pole surface hardening effect. This means that the compact magnet showed a higher coercivity than the average of its parts. Energy Dispersive X-ray spectroscopy (EDX) was used to relate the anisotropic diffusion of Dy to the obtained coercivity profile.

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