MA 23: Soft and hard permanent bulk magnets

Time: Tuesday 14:00–15:45 Location: H53

MA 23.1 Tue 14:00 H53

Nd(YCe)-based 1:12 phases – an ab intio study — •Heike C. Herper[1], Olga Yu. Vekilova[1], Alena Vishina[1], and Olle Eriksson[1,2] — [1]Department of Physics and Astronomy, Uppsala University, 75120 Uppsala, Sweden — [2]School of Science and Technology, Örebro University, 70182 Örebro, Sweden

The increase of environmental friendly energy production is coupled to an increasing demand of new magnetic materials and the identification of solutions based on abundant materials avoiding or reducing the amount of critical raw materials. In the present study we focus on the tetragonal 1:12 phase ($TmMn_{12}$ structure) which contains 35% less RE than the commercially used NdFeB compounds. Aiming to tune the magnetic performance towards large magneto crystalline anisotropy and high Curie temperatures systematic ab initio calculations have been performed. Starting from $NdFe_{11}Z$ the dependence of the magnetic performance on the type and concentration of the phase stabilizing element Z has been studied. To further reduce the RE concentration simultanously possible replacements for Nd were tested. A large composition range was found to be stable and especially doping on the RE site turned out to be suitable.

The systems were characterized using a combination of different state of the art first principles methods (VASP, RSPt). Finite temperature properties were obtained from mapping the system on a spin model using UppASD.

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MA 23.2 Tue 14:15 H53

***Ab initio* Study of Magnetic Properties of Rare-Earth lean 1:12 Alloys** — •Olga Vekilova[1], Olle Eriksson[1,2], and Heike C. Herper[1] — [1]Department of Physics and Astronomy, Uppsala University — [2]School of Science and Technology, Orebro University

Since the discovery of $Nd_2Fe_{14}B$, the best permanent magnet to date, magnets containing the combination of rare earth elements and Fe attract high scientific interest. The iron-rich compounds are specifically attractive as they have large magnetic moments due to the high concentration of Fe, rather high coercivity and high Curie temperature. One of the best candidates are the 1:12 compounds with the $ThMn_{12}$-type structure. It has been shown that light rare earths and iron cannot form a stable binary 1:12 compound, so a third element must be added to stabilize the ternary $RE(Fe,M)_{12}$ phase, where M=Ti, V, Si, Mo and etc. Such substitution results in a significant decrease in the saturation magnetization and can influence magnetocrystalline anisotropy and Curie temperature of the alloy. Recent experiments show that it is possible to stabilize the 1:12 phases with reduced concentrations of M. Magnetic properties of the 1:12 compounds were studied theoretically from first principles. Starting from the known stable $SmFe_{10}V_2$ and $NdFe_{11}Ti$ we improved the magnetic properties by reducing the content of V and Ti respectively. The phase stabilities, magnetizations, Curie temperature, magnetocrystalline anisotropies of $NdFe_{12-x}Ti_x$ and $SmFe_{12-x}V_x$ were calculated and compared to the available experimental data. This work is supported by the European Research Project NOVAMAG (EU686056) and STandUP for energy (Sweden).

MA 23.3 Tue 14:30 H53

Polymer bonded 3D-printed permanent magnets: A comparison of properties — •Georgia Gkouzia[1,2,3], Tobias Braun[1], Stefan Riegg[1], Konstantin P. Skokov[1], Dimitris Niarchos[3], and Oliver Gutfleisch[1] — [1]Funktionale Materialien, Institut für Materialwissenschaft, TU Darmstadt, Alarich-Weiss-Str. 16, D-64287 Darmstadt, Germany — [2]School of Chemical Engineering, National Technical University of Athens, Iroon Polytechniou 9, Zografou 15780, Athens, Greece — [3]AMEN Technologies, Neapoleos 27 and Patr. Grigoriou, 153 10 Athens, Greece

Recent developments in additive manufacturing (3D-printing) give the possibility of production of magnet structures which are not possible to obtain by using conventional methods. 3D-printing started as a pioneering method for polymer and ceramic materials giving the opportunity of rapid prototyping. First attempts have been made now in the production of permanent magnets. In this work, we used different polymers (PLA, PA12) and commercial magnet powders (MQA, MQP-S) for the production. We compare the properties of polymer bonded magnet with magnets made by Fused Deposition Modeling (FDM) and Laser Powder-Bed Fusion (LPBF). For the comparison of these different production routes, we investigate the microstructure and magnetic properties (B_r, H_c,$(BH)_{max}$) and the density (filling ratio of the magnetic material) of the produced samples.

MA 23.4 Tue 14:45 H53

Rare-earth lean exchange spring permanent magnets — •Stefan Riegg[1], Lukas Schäfer[1], Iuliia P. Novoselova[2], Tobias Braun[1], Marina Spasova[2], Iliya Radulov[1], Corinna Müller[1], Ralf Meckenstock[2], Konstantin P. Skokov[1], Michael Farle[2], and Oliver Gutfleisch[1] — [1]Funktionale Materialien, Fachbereich Material- und Geowissenschaften, Technische Universität Darmstadt, 64287 Darmstadt, Germany — [2]Fakultät für Physik und Center for Nanointegration (CENIDE), Universität Duisburg-Essen, 47057 Duisburg, Germany

Standard high performance permanent-magnet materials are based on rare-earth element – $3d$ metal compounds such as Nd-Fe-B and Sm-Co. To increase sustainability of these magnets, a reduction of the rare-earth element content could be one target. For instance, exchange spring magnets could be a reasonable solution to this task. In this class of materials the exchange interaction of a hard- and a soft-magnetic phase leads to a simultaneously high remanence and high coercivity, although only a relatively small fraction of the hard-magnetic material is present.

A rare-earth lean Nd-Fe-B related material is commercially available as gas-atomized powder: MQP-S. The production of magnets based on this powder will be shown for different routes (Polymer bonding, 3D printing, hot compaction), and the respective stabilities of the exchange coupling behavior and coercivity will be discussed. Advanced characterization of magnetic properties as well as detailed microstructural investigations will be presented.

MA 23.5 Tue 15:00 H53

A multiscale study of antiphase boundary of the MnAl τ-phase — •Sergiu Arapan[1], Pablo Nieves[2], and Thomas Schrefl[3] — [1]IT4Innovations, VSB-Technical University of Ostrava, 17. listopadu 15, CZ-70833 Ostrava-Poruba, Czech Republic — [2]ICCRAM, International Research Center in Critical Raw Materials and Advanced Industrial Technologies, University of Burgos, 09001 Burgos, Spain — [3]Department for Integrated Sensor Systems, Danube University Krems, 2700 Wiener Neustadt, Austria

We have implemented a multiscale model to design a realistic permanent magnet material. We quantify for the first time the exchange interaction strength across the antiphase boundary (APB) defect of the MnAl τ-phase with a simple approach derived from first-principles. The calculated exchange interaction at the APB of the MnAl τ-phase is strong enough to form an APB decorated with a domain wall, as it is always observed in experiments. This result is used in micromagnetic simulations for designing a microstructure of the MnAl τ-phase with APBs that optimizes the energy density product. The link between first-principle and micromagnetic calculations is porvided by atomistic spin dynamics. The developed multiscale modelling shows that ABPs deteriorate the loop shape through nucleation of reversed domains at very low field values and successive domain wall pinning. The energy density product decreases with increasing the number of antiphase boundaries.

MA 23.6 Tue 15:15 H53

Coercivity and anisotropy measurements on $GdCo_{5-x}Cu_x$ single crystals — •Stefan Giron, Léopold V.B. Diop, Iliya A. Radulov, Konstantin P. Skokov, and Oliver Gutfleisch — TU Darmstadt, FB Materialwissenschaft, Alarich-Weiss-Str. 16, 64287 Darmstadt, Germany

Rare-earth transition-metal permanent-magnets possess remarkably high anisotropy energies and therefore may express high coercivities necessary for permanent-magnet applications. Nonetheless, coercivity is limited to approximately one third of the anisotropy field (Brown's paradox). Coercivity mechanisms driven by exchange interaction (e.g. exchange bias) recently observed in compensated bulk Heuslers [1] and Heusler segregations [2] provide the means necessary to overcome

Brown's paradox. Though not fully understood, the coexistence of FM and AFM clusters seems to be necessary in these systems. Materials with a compensation point (e.g. $GdCo_{5-x}Cu_x$ [3]) present themselves as model objects to study giant coercivity near the FM-AFM transition. We investigated a series of ferrimagnetic $GdCo_{5-x}Cu_x$ single crystals ($x \in 0.5, 1, 1.5, 2$), which traverse a composition dependent compensation point. We show that the fields needed to demagnetize the samples approach their maximum (above 14T) near the compensation point, where the respective anisotropy fields reach minimum values.

[1] Nayak et al. Nature Materials, 2015, 14, 679
[2] Çakir, Scientific Reports, 2016, 6
[3] Grechishkin et al. Applied Physics Letters, 2006, 89, 122505

MA 23.7 Tue 15:30 H53

Low-Dimensional Magnetic Properties of Natural and Synthetic Mixite (Bi,Ca)Cu6(OH)6(AsO4)3 * nH2O (n 3) and Goudeyite YCu6(OH)6(AsO4)3 * nH2O (n 3) — •Aleksandr Golubev[1], Eva Brücher[1], Armin Schulz[1], Reinhard Kremer[1], Franz Schmidt[2], Elija Gordon[3], and Myung-Hwan Whangbo[3] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Staatliches Museum für Naturkunde, Stuttgart, Germany — [3]North Carolina State University, Raleigh. USA

The minerals mixite and goudeyite with composition $(Bi,Ca)Cu_6(OH)_6(AsO_4)3{*}nH_2O(n = 3)$ and $YCu_6(OH)_6(AsO_4)_3{*}nH_2O$ (n = 3) crystallize in the space group P 6_3/m (no. 176) with a "zeolite-type" channel structure with a honeycomb arrangement of rings composed of six CuO_4 ribbon chains. The structural, vibrational and magnetic properties of natural and synthetic polycrystalline samples of the minerals mixite and goudeyite have been investigated. The magnetic susceptibilities are characterized by low-dimensional antiferromagnetic short range ordering and can be described as spin S=1/2 alternating Heisenberg chain with nearest-neighbor spin exchange ranging between 200 K and 130 K for natural mixite and synthetic goudeyite, respectively. The alternation parameters range between 0.52 for natural mixite and 0.75 for synthetic mixite and goudeyite, respectively. The experimentally observed spin exchange parameters are consistent with DFT calculations of the spin exchange parameters.