MA 50: Permanent Magnets

Time: Thursday 15:00–17:30 Location: HSZ 101

MA 50.1 Thu 15:00 HSZ 101

High-throughput and data-mining search for rare-earth free permanent magnets — •Alena Vishina[1], Olga Yu. Vekilova[1], Heike C. Herper[1], and Olle Eriksson[1,2] — [1]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — [2]School of Science and Technology, Örebro University, Örebro, Sweden

High performance permanent magnets are needed for a large number of applications, such as electric motors, wind mills, and many more. At the same time most high performance magnets contain rare-earth (RE) materials which makes them expensive, while some of the RE elements are rapidly decreasing in availability.

We've applied a high-throughput and data-mining approach to the search of rare-earth free permanent magnets. Going through a large number of known structures from ICSD database, and using a full-potential linear muffin-tin orbital method with relativistic formulation as implemented in the RSPt electron structure code to calculate magnetic anisotropy and Curie temperature, we were looking for the materials with high magnetization > 1 T, uniaxial anisotropy > 1 MJ/m^3, and $T_c > 300$ K to identify the suitable replacement for rare-earth containing materials.

Starting with the materials containing 3d+5d+1 extra element of the periodic table to test the method, we have found several candidates that have characteristics suitable for a good permanent magnet, such as Pt_2FeCu, Pt_2FeNi, W_2FeB_2, etc (arXiv:1910.00548 [cond-mat.mtrl-sci]).

MA 50.2 Thu 15:15 HSZ 101

Computational design of rare-earth lean hard magnetic phases — •Heike C. Herper[1], Olga Yu. Vekilova[1], Pablo Nieves[2], and Olle Eriksson[1,3] — [1]Department of Physics and Astronomy, Uppsala University, Sweden — [2]T4Innovations, VŠB Technical University of Ostrava, Czech Republic — [3]School of Science and Technology, Örebro University, Sweden

Today nearly all high performance magnets are based on $Nd_2Fe_{14}B$ and the demand for such magnets is increasing. Thus more permanent magnets are needed but the new materials should have a smaller environmental footprint. Fe-rich phases with the $ThMn_{12}$ structure contain less RE than the commercially used compounds.

We performed a systematic ab initio study of $REFe_{12-x}Z_x$ with RE = Nd, Y, Ce, Sm; Z = Ti, V aiming to tune the magnetic performance towards large uniaxial magnetocrystalline anisotropy and high T_C by using a combination of different state of the art first principles methods combined with atomistic simulation methods for temperature dependent properties. Apart from Sm in practice N must be added to e.g. improve the coercive field. Since especially N can alter the orientation of the easy axis it has been included in the study.

Several promising phases could be identified. Here, $YFe_{11.5}Ti_{0.5}N$, and $Nd_{0.5}Y_{0.5}Fe_{11}Ti(N)$, and $SmFe_{11}V$ will be discussed. The last one has been already synthesized showing an good magnetic performance.[J. Alloys and compounds **786**, 969 (2019)]
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MA 50.3 Thu 15:30 HSZ 101

Computational screening of Fe-Ta magnetic phases — •Sergiu Arapan[1], Pablo Nieves[1], Heike C. Herper[2], and Dominik Legut[1] — [1]IT4Innovations, VŠB - Technical University of Ostrava, 17. listopadu 15, 70833 Ostrava-Poruba, Czech Republic — [2]Department of Physics and Astronomy, Uppsala University, Box 516, 75121 Uppsala, Sweden

In this work we perform a systematic calculation of the Fe-Ta phase diagram. Despite of the fact that the two experimentally observed ordered Fe-Ta alloy phases do not exhibit magnetic properties suitable for permanent magnets (PMs), our computational study suggests that new phases, with intrinsic magnetic properties appropriate for PMs, might exist within this binary system. By using structure prediction methods based on evolutionary algorithms and density functional theory, we identify two energetically stable magnetic structures: a tetragonal Fe_3Ta (space group 122) and a cubic Fe_5Ta (space group 216) binary phases. The tetragonal structure is estimated to have both high saturation magnetization ($\mu_0 M_s$=1.14 T) and magneto-crystalline anisotropy (K_1=2.17 MJ/m^3) suitable for permanent magnet applications. In addition, we discover two metastable hard magnetic phases: Fe_5Ta_2 (space group 156) and Fe_6Ta (space group 194), that may exhibit intrinsic magnetic properties comparable to $SmCo_5$ and $Nd_2Fe_{14}B$, respectively. From the results of electronic structure calculations we determine electronic states responsible for such large MAE and identify a criterion to find hard magnetic structures in rare-earth free intermetallic systems.

MA 50.4 Thu 15:45 HSZ 101

Strong magnetocrystalline anisotropy and magnetic hardness at room-temperature in the rare-earth-free magnet Rh2CoSb — •Yangkun He[1], Gerhard Fecher[1], Rudolf Schaefer[2,3], S. S. P. Parkin[4], J. M. D. Coey[5], and Claudia Felser[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]Institute for Materials Science, TU Dresden, D-01062 Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Helmholtzstrasse 20, D01069 Dresden, Germany — [4]Max Planck Institute of Microstructure Physics, Halle, Germany — [5]School of Physics, Trinity College, Dublin 2, Ireland

Strong uniaxial magnetocrystalline anisotropy is indispensable for a permanent magnet, but it is rarely achieved in rare-earth-free compounds. Here we report a magnetocrystalline anisotropy of 3.62 MJm-3 in single crystals of a tetragonal Heusler compound Rh2CoSb with a saturation magnetization of μ0Ms = 0.52 T at 2 K (2.20 MJm-3 and 0.44 T at room-temperature). The magnetic hardness parameter κ of 3.7 at room temperature is the highest observed for a rare-earth-free magnet. Strong anisotropy is also manifest in the transport properties; the values of electrical and thermal conductivities are twice as large along the c axis as along the a axis and there are significant differences of the anomalous Hall effect and magnetoresistance. Our study illustrates the benefits of designing highly anisotropic rare-earth-free magnets using 4d elements, with potential as future thin film media.

MA 50.5 Thu 16:00 HSZ 101

Influence of cooling conditions and alloy composition on the microstructure of NdFeB alloys for a deformation production route — •Corinna Müller[1], Franziska Staab[1], Fansun Chi[2], Peter Groche[2], Enrico Bruder[3], Karsten Durst[3], Stefan Riegg[1], and Oliver Gutfleisch[1] — [1]Funktionale Materialien, FB Materialwissenschaft, TU Darmstadt — [2]Institut für Produktionstechnik und Umformmaschinen, FB Maschinenbau, TU Darmstadt — [3]Physikalische Metallkunde, FB Materialwissenschaft, TU Darmstadt

NdFeB permanent magnets play a key role in renewable energy technologies because their use is required for efficient electric machines. The specific microstructure of these magnets is directly connected to their magnetic performance. The classical powder metallurgical production route uses jet milling and sintering to achieve homogeneous grain sizes of a few micrometers. The related processing costs are however rather high and the here introduced use of rotary swaging could be an alternative and cheaper technique, allowing continuous processing. During swaging in this top-down processing approach the grain size of a cast body is reduced by the deformation. In this work, experiments to microstructure optimization of the starting alloy precursor after casting are presented and compared to the classical powder metallurgical processing. The microstructure was manipulated by the casting mold geometries and the addition of different dopants. The aim is to understand the thermodynamic and kinetic properties of the process (cooling conditions, phase formation, size distribution) and derive an adequate starting microstructure for rotary swaging.

15 min. break.

MA 50.6 Thu 16:30 HSZ 101

Magnetic properties of "1-5" intermetallic compounds from first principles — •Olga Vekilova[1], Heike C. Herper[1], and Olle Eriksson[1,2] — [1]Uppsala University, Uppsala, Sweden — [2]Örebro University, Örebro, Sweden

Permanent magnets are of vital importance for sustainable industry and in particular, are parts of most of the sources of "green" energy. The $RECo_5$, so-called "1-5" intermetallic compounds with the hexagonal $CaCu_5$ structure, where RE represents the rare-earth elements, such as Ce, Sm, Gd, etc., have been attracting attention primarily due

to their excellent magnetic properties. These magnets exhibit very high value of magnetocrystalline energy (MAE), the key intrinsic property for the applications[1]. However theoretical studies of $RECo_5$ are very limited due to difficulties in the description of localized 4f-states of RE-elements. One of the well-known examples is $GdCo_5$, where the symmetry of the Gd 4f shell causes crystal field effects to vanish [2]. The absence of crystal-field effects makes $GdCo_5$ a particularly useful system to study the rare-earth/transition-metal interaction via both theory and experiment. This system also has relatively high MAE, which can be further improved by doping and pressure. Using our improved theoretical methodology, we studied the magnetic properties of pure and doped 1-5 compounds. The results on magnetization, MAE, and Curie temperature will be presented and analyzed. We will also show how doping of $RECo_5$ allows changing of its magnetic properties in a controlled manner. [1] J. Phys.: Condens. Matter 30 195801 (2018) [2] Phys. Rev. Materials 3, 034409 (2019)

MA 50.7 Thu 16:45 HSZ 101

Interplay between chemical order and magnetic properties in $L1_0$ FeNi (tetrataenite): A First-Principles Study — •Ankit Izardar and Claude Ederer — Materials Theory, ETH Zuerich, Switzerland

The volatility in price and uncertainty of supply of rare earth elements has sparked great interest to explore permanent magnets that are free from rare-earth elements. One interesting candidate in this quest is a chemically-ordered $L1_0$ $Fe_{50}Ni_{50}$ found in iron meteorites. However, laboratory synthesis of the ordered phase is extremely challenging because of the slow diffusion of atoms at the rather low order-disorder transition temperature. Until now, only partially ordered samples have been synthesized. Therefore, it is important to know how deviations from perfect chemical order affect the magnetic properties.Using first-principles-based density-functional theory calculations in combination with Monte Carlo (MC) simulations, we investigate the interplay between chemical order and the magnetic properties of the $L1_0$ FeNi phase. We use a supercell approach to model structures with varying degree of chemical order in combination with the disordered local moment method to describe the paramagnetic state. Our calculations demonstrate a strong effect of the magnetic order on the chemical order-disorder transition temperature and vice-versa. Furthermore, we also investigate dependence of the magneto-crystalline anisotropy (MAE) on the chemical long range order. Our results indicate that small deviations from perfect order do not significantly decrease the MAE with respect to a completely ordered FeNi alloy.

MA 50.8 Thu 17:00 HSZ 101

Impact of magnetism on the phase stability of rare-earth based hard magnetic materials — •Halil Ibrahim Sözen, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

In recent years, quantum-mechanically guided materials design has been successfully used to identify candidate hard magnetic materials with a reduced content of rare earth elements. These studies were restricted to identify optimal magnetic properties. In the present work we address the issue of thermodynamic stability of such materials, i.e., whether such materials can be actually formed. As prototype system we consider CeFe11Ti and focus on the impact of magnetism on the free energy. To this end, we use the magnetic model suggested by Gerhard Inden as a reference. The performance of this model is compared to Monte Carlo simulations for the magnetic entropy contribution. We conclude that despite the empirical nature of the Inden model, it provides a surprisingly accurate description of the magnetic contribution. Based on this approach we are able to faithfully predict the critical temperature for the decomposition of CeFe11Ti into competing Laves phases. We further show that the Inden model can be improved if the reduction of the magnetic moment at finite temperatures is taken into account. This is demonstrated for the hard magnetic phase Nd2Fe14B. In addition, the impact of magnetism on the lattice vibrations of relevant phases in the Ce-Fe-Ti system is analyzed.

MA 50.9 Thu 17:15 HSZ 101

Manipulation of intrinsic properties of $CeFe_{11}Ti$: Experiment and Theory — •Semih Ener[1], Anna Galler[2], Fernando Maccari[1], Imants Dirba[1], Konstantin P. Skokov[1], Silke Biermann[2], Leonid Pourovskii[2], and Oliver Gutfleisch[1] — [1]Functional Materials, Department of Materials Science, Technische Universität Darmstadt, Darmstadt/Germany — [2]Centre de Physique Théorique, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau/France

The abundance of rare-earth (RE) elements like Nd and Sm motivates researchers to look for alternative free-RE (like Ce, Pr, La) material systems. Interesting candidates are $ThMn_{12}$-phases where the RE concentration is lower in comparison to the benchmark material systems $Nd_2Fe_{14}B$ and Sm_2Fe_{17}. The $CeFe_{12}$ phase is not stable in bulk form, so additional elements need to be substituted for Fe to stabilize the phase. Among the alternative stabilization elements, titanium is a promising candidate due to its low composition ratio (approx. 7 at.% for stabilization of the $ThMn_{12}$-phase in bulk) for ternary concentrations. In this work, we carried out composition and thermal treatment optimization for the $Ce_{1+x}Fe_{11}Ti$ series and investigated the magnetic properties under positive and negative pressures. In addition to the experiments, first-principles dynamical mean-feld theory (DMFT) calculations were carried out. Intrinsic properties were investigated at different temperatures and will be presented in this work.

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