# MA 56: Bulk Materials: Soft and hard permanent magnets

Time: Thursday 15:00–18:00 Location: HSZ 403

MA 56.1 Thu 15:00 HSZ 403

**Ab initio theory of Fe-based permanent magnets** — •Olga Vekilova, Olle Eriksson, and Heike Herper — Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Strong permanent magnets are of great importance for many technological applications, from magnetic resonance imaging to green sources of energy. The modern society is currently interested in the design of magnetic materials that are cheaper and contain smaller amounts of rare earth elements compared with the existing ones. Theoretical modelling is a promising tool to discover new advanced rare earth-free permanent magnets. Good permanent magnet is a ferromagnetic compound with high Curie temperature, high saturation magnetization and high anisotropy energy. The latter is the key factor for the required large coercivity and in addition it should be uniaxial. The listed conditions are satisfied in Fe-rich materials, in particular in hexagonal $Fe_3Sn$. However, as it is known from both the experiment and the theory, the easy magnetization axis lies in the hexagonal plane. One of the possibilities for changing the easy axis direction is through alloying. We have studied the magnetic properties of Fe-based alloys with phase stabilizers, such as Sn, Sb, Ga, Ge and Si to find new ferromagnetic phases with uniaxial anisotropy suitable for the development of advanced permanent magnets. The calculated magnetocrystalline anisotropies and Curie temperatures of these compounds are analyzed and suggestions for the better permanent magnets are formulated. The work is supported by NOVAMAG (EU686056)

MA 56.2 Thu 15:15 HSZ 403

**The influence of the Madelung potential on magnetic properties of disordered FePt** — •Saleem Ayaz Khan[1], Peter Blaha[2], Hubert Ebert[3], Jan Minár[1,3], and Ondřej Šipr[1,4] — [1]New Technologies Research Centre University of West Bohemia, Pilsen, Czech Republic — [2]Institute of Materials Chemistry, TU Vienna, Austria — [3]Universität München, Department Chemie, Germany — [4]Institute of Physics ASCR v. v. i., Prague, Czech Republic

When dealing with substitutional alloys, the random occupation of sites has to be approximated. One can use supercells to include many different local configurations. Or one can rely on a mean field method such as the coherent potential approximation (CPA) to model the situation by an auxiliary effective medium. Computationally efficient single site CPA treats the disorder itself very efficiently. However, being a single-site method, it neglects the effect of fluctuations of the local environment. In particular, the Madelung contribution to the alloy potential cannot be included within the standard CPA.

To learn more about the local aspects of magnetism of disordered FePt, we performed a set of ab-initio relativistic full-potential calculations employing both the supercell approach and the CPA. The focus is on the trends of local magnetic moments with the chemical composition of the nearest neighbourhood of individual Fe and Pt atoms. A small but distinct difference between average magnetic moments obtained when using the supercells and when relying on the CPA is identified and linked to the neglect of the Madelung potential in the CPA.

MA 56.3 Thu 15:30 HSZ 403

**Grain boundary diffusion of different rare earth elements in Nd-Fe-B sintered magnets by experiment and FEM simulation** — •Konrad Loewe[1], Dimitri Benke[1], Christian Kübel[2], Konstantin Skokov[1], and Oliver Gutfleisch[1] — [1]TU Darmstadt, FB Materials Science, 64287 Darmstadt — [2]KIT, Institute of Nanotechnology & Karlsruhe Nano Micro Facility, Hermann-von-Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

In the present work, we explore the influence of a surface-bulk coercivity gradient in Nd-Fe-B magnets produced by the Grain Boundary Diffusion Process (GBDP) on the overall coercivity. In our systematic and comprehensive study we diffused four different rare earth elements (Dy, Tb, Ce and Gd) in two different kinds of commercial Nd-Fe-B magnets, one very Dy-lean and one Dy-rich. By means of cutting the magnets into thin slices we obtain lateral coercivity profiles, from which diffusion constants are extracted. We find that in both magnets Tb diffuses significantly faster than Dy. Ce diffuses slightly slower than Dy and the overall coercivity decrease is similar for Ce and Gd. High-resolution scanning transmission electron microscopy shows the nano-scale distribution of Tb around the grain boundaries located in the bulk of the magnet. Finally, a simple model for the magnetization reversal in grain boundary diffusion processed gradient Nd-Fe-B magnets was developed and implemented into a FEM software. Our calculated demagnetization curves correspond very well for the Dy and Tb samples, but deviate significantly for Ce and Gd.

MA 56.4 Thu 15:45 HSZ 403

**Reliability of bulk combinatorial reactive crucible melting approach to search for new permanent magnets: a Fe-Sn case study** — •Bahar Fayyazi, Konstantin Skokov, Dmitriy Karpenkov, and Oliver Gutfleisch — Technical University of Darmstadt

The search for new magnetic materials using conventional equilibrated alloy methods is an expensive and time-consuming task. Therefore, high-throughput methods where multiple alloy compositions (material libraries) can be synthesized and characterized together would be a powerful tool. Reactive crucible melting (RCM) as well as diffusion couple/multiple approach are potential bulk high-throughput methods in order to speed up the discovery and examination of new materials. However, in previous investigations [1] by diffusion multiple approach, it has been found that under specific conditions there may exist some phases which are not forming by interdiffusion reactions. This assessment motivated us to evaluate whether a similar situation may occur in RCM method. Therefore, a detailed study has been conducted on the simple and well-studied Fe-Sn binary system by correlating the forming phases in reactive crucible samples to the known phase diagram. Simultaneously, under the same conditions as for the crucibles, 10 individual homogeneous samples were prepared by conventional metallurgy and the results were compared to RCM samples. Discrepancies which have been observed will be discussed in this work.

[1] J.C. Zhao, Reliability of the diffusion-multiple approach for phase diagram mapping, J. Mater. Sci., 39 (2004) 3913-3925.

MA 56.5 Thu 16:00 HSZ 403

**Ferromagnetism vs. slow relaxation in Fe-doped $Li_3N$** — •Manuel Fix[1], Rudra S. Manna[1], Stephan G. Jantz[2], and Anton Jesche[1] — [1]EP 6, Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Solid State Chemistry, Insitute of Physics, University of Augsburg, Germany

The compounds $Li_2(Li_{1-x}T_x)N$ where $T = \{Mn, Fe, Co and Ni\}$ show a highly anisotropic behaviour of their magnetic properties resulting from large orbital contributions to the magnetic moment of the transition metals [1,2]. In the case of Fe-doping, this results in a huge magnetic hysteresis with coercive fields of more than 11 T, tempting one to claim a ferromagnetic behaviour in the compound. On the other hand, $Li_2(Li_{1-x}Fe_x)N$ shows a pronounced time dependence of the magnetization, reminiscent of spin glasses or molecular magnets.

We will discuss the intriguing magnetic properties of $Li_2(Li_{1-x}Fe_x)N$. Isothermal magnetisation curves will be compared to direct measurements of the magnetic relaxation, as well as the frequency dependence of the ac-susceptibility. Furthermore, similarities between the hysteresis in magnetization and magnetostriction are going to be discussed.

[1] A. Jesche *et al.*, Phys. Rev. B **91**, 180403(R) (2015)
[2] A. Jesche *et al.*, Nature Comm. **5**:3333 (2014)

MA 56.6 Thu 16:15 HSZ 403

**Producing two different $L1_0$ phases in ternary MnAlGa alloys** — •Torsten Mix[1,2], Florian Bittner[1,3], Karl-Hartmut Müller[1], Ludwig Schultz[1,2,3], and Thomas George Woodcock[1] — [1]IFW Dresden, Institute for Metallic Materials, PO Box 270116, 01171 Dresden, Germany — [2]Department of Physics, TU Dresden, Dresden, Germany — [3]Institute for Materials Science, TU Dresden, Dresden, Germany

The $L1_0$ phases in the binary MnAl and MnGa systems are interesting candidates for rare earth free permanent magnets. The main drawbacks, are the high price of Ga and the poor resistance to decomposition at evelated temperature of the metastable $L1_0$ phase in binary MnAl. As the $L1_0$ phase in MnGa is thermodynamically stable, the

formation of a ternary MnAlGa alloy is a promising approach to overcome these difficulties. Ternary alloys of the form $Mn_{55}Al_{45-x}Ga_x$ have been produced in the range $0 < x < 45$. In alloys with $5 < x \leq 9$ after appropriate heat treatments, two different phases with the $L1_0$ structure can be made to coexist. One is stable as in the binary MnGa system, the other metastable as in binary MnAl. The magnetic properties of the ternary alloys are superior to those of the binary analogues. The thermal stability of the metastable phase is greatly improved by the addition of the small amount of Ga. Up to 700°C, the decomposition of the metastable phase is strongly suppressed. This allows longer processing time at higher temperatures, thus enabling new routes to produce rare earth free MnAl-based magnets to be envisaged.

**15 min. break.**

MA 56.7 Thu 16:45 HSZ 403

**Impact of dislocations on coercivity in $L1_0$-MnAl** — •Florian Bittner[1], Jens Freudenberger[1,2], Ludwig Schultz[1], and Thomas G. Woodcock[1] — [1]IFW Dresden, Institute for Metallic Materials, PO Box 270116, 01171 Dresden, Germany — [2]TU Bergakademie Freiberg, Institute of Materials Science, Gustav-Zeuner-Straße 5, 09599 Freiberg, Germany

Novel rare-earth free hard magnetic compounds are of growing interest due to the demand for permanent magnets with maximum energy densities between those of ferrites and rare earth magnets. The $L1_0$ ordered $\tau$-MnAl is one candidate material for applications due to its promising intrinsic magnetic properties. Even though the anisotropy field is approximately 5 T, the coercivity achieved in bulk magnets is currently too low to reach its full potential. The reason for this discrepancy is caused by the microstructure of the material and the impact microstructural features on the magnetic properties. The coercivity of cold worked $Mn_{54}Al_{46}$ is remarkably increased from 0.02 T in the initial state to 0.29 T. Further annealing reduces coercivity while the microstructure remains unchanged within the resolution limit of the scanning electron microscope. Direct analysis of the quality of electron backscatter diffraction patterns was used to approximate the local dislocation density in the materials. The results showed significant evidence for different dislocation densities in the different metallurgical conditions. The conclusion that dislocations can act as pinning sites is also supported by the shape of the initial magnetisation curve and explained by local changes of the intrinsic magnetic properties.

MA 56.8 Thu 17:00 HSZ 403

**A systematic study of RE lean $ThMn_{12}$-type phases** — •Heike C. Herper, Olga Vekilova, and Olle Eriksson — Department of Physics and Astronomy, Uppsala University, Sweden

The demand for high performance magnets increases with the increasing usage of renewable energies, e.g. wind power plants. New magnets with lower content of rare earth (RE) compared to todays Fe-Nd-B magnets are needed. Rare earth lean systems such as $REFe_{12-x}M_x$ in the $ThMn_{12}$ structure are viewed as good alternatives because their RE content is much smaller and high anisotropies can be reached with interstitial nitrogen atoms. Even though these systems have been investigated for years systematic only few systematic studies exist which analyze the dependence of the magnetic properties on the concentration of the stabilizing element and the optimal N content in detail.

Here a series of $REFe_{12-x}M_xN_y$ phases with M = Ti, V and RE = Nd and Y has been systematically investigated with density functional theory methods in view of phase stability and magnetic properties depending on the amount of M and N. The geometry has been optimized using the VASP code and magnetic properties have been calculated within the full potential LMTO code RSPt [1] treating the 4f electron as a spin-polarized core electron.

[1] J. M. Wills et al, Full-Potential Electronic Structure Method, Vol. **167**, Springer series in solid state science (2010).

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MA 56.9 Thu 17:15 HSZ 403

**High-throughput density functional screening for permanent magnet materials** — •Ingo Opahle — TU Darmstadt, Germany

High-throughput density functional calculations are used to search for candidates for new rare earth free permanent magnet materials. The key quantity here is the magneto-crystalline anisotropy energy (MAE), which sets an upper bound to the coercivity. The concept is explained at hand of the well-known Co-Pt system. It is shown that a considerably higher MAE than in the known L10 structure is possible, provided meta stable crystal structures can be stabilized, e.g by addition of a suitable element. Applications to further systems will be shown as well.

MA 56.10 Thu 17:30 HSZ 403

**Magnetization behavior of hexagonal ferrites observed by *in-situ* Magnetic Force Microscopy** — •Tim Helbig[1], Fabian Rhein[2], Volker Neu[3], Michael Krispin[2], and Oliver Gutfleisch[1] — [1]TU Darmstadt — [2]Siemens AG — [3]IFW Dresden

The sintering temperature of hexagonal ferrites with increasing partial Al substitution was systematically varied to obtain different microstructures. The grain size was found to range from a few hundred nanometers to several hundred micrometers. The grain size distribution depended on the Al content as well as the pre-milling and sintering conditions. Magnetic Force Microscopy (MFM) showed that the microstructure consists of a mixture of grains below the critical single-domain size, and larger grains with a multi-domain structure in the thermally demagnetized state (TDS). An *in-situ* MFM study was carried out depicting the magnetization from the TDS as well as the demagnetization under external magnetic field. From the surface domain contrast a magnetization was derived which quantitatively matches the global i.e. bulk magnetization obtained by SQUID magnetometry. The shape of the initial magnetization curve and the magnetization from the DC demagnetized state was correlated with the *in-situ* MFM data revealing a distinctly different magnetization behavior depending on grain size. Financial support by the German federal state of Hessen through its LOEWE program "RESPONSE" is gratefully acknowledged. The material development has been performed in BMBF funded project KomMa (03X3582).

MA 56.11 Thu 17:45 HSZ 403

**Neutron depolarization imaging of magnetite in chiton teeth** — •Marc Seifert[1,2], Michael Schulz[1,2], Georg Benka[2], Christian Pfleiderer[2], and Stuart Gilder[3] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, D-85748 Garching, Germany — [2]Physics Department, Technical University of Munich, D-85748 Garching, Germany — [3]Department of Earth and Environmental Sciences, Ludwig-Maximilians-Universität München, D-80539 Munich, Germany

Magnetite constitutes one of the most abundant magnetic minerals in the Earth's crust. In the single domain state, magnetite often carries the magnetic remanence in rocks due to its stable and strong magnetic remanence. Hence it is of keen interest to paleomagnetists who study the ancient magnetic field preserved in the rock record. The extremely small size range and vulnerability to oxidation of single domain magnetite makes synthetization and preservation virtually impossible. Consequently, most experimental work on magnetite under pressure is carried out on multidomain magnetite. The radula of the marine mollusc chiton (Polyplacophora) is one of the few natural sources of single domain magnetite. We have performed a comparative study on samples of chiton radula in a vibrating sample magnetometer (VSM) and with the newly evolving neutron depolarization imaging (NDI) technique. Despite a constant offset between the VSM and NDI data in the coercivity we find a good agreement between the two techniques.