MA 24: Magnetic Materials I

Time: Wednesday 9:30–12:30 Location: H 0112

MA 24.1 Wed 9:30 H 0112

Excitations in the Skyrmion Lattice of the Molecular Magnet GaV_4S_8 — •Dieter Ehlers[1], Vladimir Tsurkan[1], Hans-Albrecht Krug von Nidda[1], István Kézsmárki[2], Ioannis Stasinopoulos[3], Dirk Grundler[3], and Alois Loidl[1] — [1]Experimentalphysik V, EKM, Universität Augsburg, 86135 Augsburg — [2]Department of Physics, Budapest University of Technology and Economics, 1111 Budapest, Ungarn — [3]Physik-Department E10, TU München, 85747 Garching

The magnetic semiconductor GaV_4S_8 has the so-called lacunar spinel structure which can be derived from the normal spinel structure by removing every second Ga atom. On cooling, a Jahn-Teller instability lowers the symmetry from cubic to trigonal at 44 K, resulting in twinned crystals. Magnetism arises from V_4S_8 clusters[1,2] which carry an effective spin $\frac{1}{2}$, and leads, below 13 K, to a complex magnetic phase diagram consisting of cycloidal, skyrmion, and ferromagnetic regions. These are interpreted in terms of a competition of anisotropic exchange coupling as well as Zeeman interactions in the multi-domain phase. Electron spin resonance has been applied to get insight into the magetization dynamics. Fixed frequency measurements prove the assumed anisotropy model and provide information on the interaction strengths. Broadband microwave experiments at low temperatures show excitations at 5 GHz and above 15 GHz, indicating that the ferromagnetic phase is more complex than anticipated so far.

[1]R. Pocha et al., Chem. Mater. **12** (2000), 2882
[2]H. Nakamura et al., J. Phys.: Condens. Matter **17** (2005), 6015

MA 24.2 Wed 9:45 H 0112

Pressure and temperature dependent powder diffraction studies on magnetocaloric compounds of the series Mn5-xFexSi3 — •Paul Hering[1], Karen Friese[1], Thomas Brückel[1], Anatoliy Senyshin[2], Michael Hanfland[3], Andrzej Grzechnik[4], Mohammad Maswada[1], and Ye Cheng[1] — [1]JCNS-2/PGI4, Forschungszentrum Jülich GmbH — [2]MLZ, TUM, Garching — [3]Inst. of Crystallo., RWTH Aachen — [4]ESRF, Grenoble, France

Magnetic refrigeration based on the magnetocaloric effect hold a potential to replace conventional vapor compression cooling. Compared to other magnetocaloric materials, the compounds in the system Mn5-xFexSi3 have the advantage that they do not contain expensive rare earth elements like Gd, nor toxic elements like As. The compounds undergo a variety of magnetic phase transitions at different temperatures depending on the iron content [Songlin, et al., J. Alloys Comp. 334, 249-252 (2002)]. Therefore, this system is an ideal choice to gain a better understanding of the underlying mechanism of the MCE in multiple site driven magnetocaloric materials. We performed neutron and x-ray powder diffraction experiments as a function of temperature and could trace several magnetic and structural transitions through anomalies in the lattice parameter showing a close connection between lattice and spin degrees of freedom. Recent synchrotron powder experiments varying pressure and temperature simultaneously were performed to elucidate, -first- whether the influence of hydrostatic and 'chemical pressure' (i.e. through the variation of composition) is equivalent, and -second- to follow the magnetic and associated structural transitions.

MA 24.3 Wed 10:00 H 0112

Element-resolved thermodynamics of $LaFe_{13-x}Si_x$ — •Markus Ernst Gruner[1,2,3], Werner Keune[2,4], Beatriz Roldan Cuenya[5], Claudia Weis[2], Joachim Landers[2], Sergey I. Makarov[2], David Klar[2], Michael Y. Hu[6], Ercan E. Alp[6], Jiyong Zhao[6], Maria Krautz[1], Oliver Gutfleisch[7], and Heiko Wende[2] — [1]IFW Dresden — [2]Universität Duisburg-Essen — [3]Forschungs-Neutronenquelle FRM II, Garching — [4]MPI Halle — [5]Ruhr-Universität Bochum — [6]Argonne National Laboratory — [7]TU Darmstadt

By combination of two independent approaches, nuclear resonant inelastic X-ray scattering and first-principles calculations in the framework of density functional theory, we demonstrate an unusual and significant effect of the magnetic phase transition on the element-resolved vibrational density of states of $LaFe_{13-x}Si_x$. This comprises the disapperance of a high-energy peak in connection with an overall softening of phonons in the paramagnetic phase, which is unexpected due to the large volume decrease at the transition. The pronounced magnetoelastic effect originates from adiabatic electron phonon coupling caused by specific changes in the electronic density of states at the Fermi level arising from the itinerant electron metamagnetism of Fe. The increase in lattice entropy associated with the Fe subsystem is significant and contributes cooperatively with the magnetic and electronic entropy changes to the excellent magneto- and barocaloric properties.

MA 24.4 Wed 10:15 H 0112

The magnetocaloric effect in transition metal borides — •Maximilian Fries[1], Konstantin Skokov[1], Michael Kuzmin[2], Zsolt Gercsi[3], and Oliver Gutfleisch[1] — [1]Technische Universität Darmstadt — [2]Faculté des Sciences et Techniques Marseille — [3]Trinity College Dublin

Magnetic cooling is a thriving research topic because it may offer considerably higher energy efficiency compared to traditional vapor compression based machines. In a reverse process the magnetocaloric effect can also be utilized in a thermoelectric generator. In order to make these technologies viable, material compositions with highly tunable Curie Temperatures (T_C) in the range of 200-600K are needed.

The group of transition metal borides may be a good candidate especially for high temperature applications, as they are chemically inert and stable in air even at elevated temperatures. Many Borides exhibit high magnetic moments for example like pure MnB which exhibits the highest magnetization of all 3d metal monoborides with 158 emu/g.

Here we will report on transition metal borides based on Cobalt, Manganese and Iron. We will show and discuss the magnetic, magnetocaloric and structural properties including spontaneous magnetization, entropy change and lattice expansion. The results are complemented with insights from theory based on DFT calculations.

MA 24.5 Wed 10:30 H 0112

Direct measurements of the magnetocaloric effect in thin film and low volume samples — •Jago Döntgen[1], Jörg Rudolph[1], Tino Gottschall[2], Oliver Gutfleisch[2], Steffen Salomon[3], Alfred Ludwig[3], and Daniel Hägele[1] — [1]AG Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, Germany — [2]Functional Materials, TU Darmstadt, Germany — [3]Werkstoffe der Mikrotechnik, Ruhr-Universität, Bochum, Germany

We present the first temperature dependent measurements of the magnetocaloric effect in a Gd thin film with sub-mK resolution. The high sensitivity of our newly developed technique of magnetomodulation combined with detection of the sample's thermal radiation allows the systematic investigation of thin film material libraries grown on wafers and gives new insights into the low-field behaviour of the magnetocaloric effect, which is not accessible by traditional calorimetry.

At T_C, we find a quadratic magnetic field dependence of the magnetocaloric ΔT for low external fields, contradicting earlier predictions. The same behaviour is found in bulk Gd and the metamagnetic alloy $LaFe_{11.05}Co_{0.91}Si_{1.04}$, underlining the versatility of our approach. An analytic expression based on Landau theory is found, that describes the transition of ΔT from the H_{ext}^2 behaviour at low to the well-known $H_{ext}^{2/3}$ behaviour at high fields.

15 min. break

MA 24.6 Wed 11:00 H 0112

Enhancement of soft magnetic properties of FeCoBSiNb bulk glassy alloys — •Parthiban Ramasamy[1], Mihai ' Stoica[2], and Jürgen Eckert[3] — [1]IFW Dresden, Institute for Complex Materials,Dresden, Germany — [2]IFW Dresden, Institute for Complex Materials,Dresden, Germany — [3]IFW Dresden, Institute for Complex Materials,Dresden, Germany

Fe based bulk metallic glasses are gaining more importance in recent decades due to their high strength and excellent soft magnetic properties, combined with low materials cost. The effect of Zr addition on the glass forming ability (GFA) of FeCoBSiNb glassy alloys in [(Fe0.5Co0.5)B0.2Si0.05]96-xNb4Zrx and [(Fe0.5Co0.5)B0.2Si0.05]100-xZrx system is investigated. In this study effect of Zr addition is studied because of its mixing enthalpies between Zr and Fe, Co, B, or Si atomic pairs are-26, -41, -49, -56, and -67 kJ/mol, respectively, and they are larger than those between Nb and Fe, Co, B, or Si atomic pairs, which are -16, -25, -30, -39, and-39

kJ/mol, respectively. The addition of Zr instead of Nb decreases the liquidus temperature of the system around 100K (i.e. from 1475K to 1370K). Thought the formation of the ZrB2 slightly affects the glass forming ability of the alloy, the Zr helps in the precipitation of (Fe, Co) phase, which is magnetically softer than the Fe23B6 phase and also mechanical properties of the alloy is improved.

MA 24.7 Wed 11:15 H 0112

Effect of particle refinement and grain boundary diffusion process in hot-deformed Nd-Fe-B permanent magnets — •Simon Sawatzki[1], Christian Kübel[2], Semih Ener[1], Imants Dirba[1], and Oliver Gutfleisch[1,3] — [1]TU Darmstadt, Materialwissenschaft, Alarich-Weiß-Str. 16, 64287 Darmstadt, Germany — [2]KIT, institute of Nanotechnology INT, P.O. Box 3640, 76021 Karlsruhe, Germany — [3]IWKS Hanau, Fraunhofer-Projektgruppe für Wertstoffkreisläufe und Ressourcenstrategie, 63457 Hanau, Germany

The grain boundary diffusion process (GBDP) drastically increases the coercivity in sintered Nd-Fe-B magnets without losing much in remanent magnetization by using only a very small amount of Dy [1]. Here Nd-Fe-B melt-spun ribbons have been hot-compacted and die-upset together with low melting DyCu, DyNdCu and TbNdCu powders to enhance coercivity. In order to optimize the distribution of these eutectics within the sample, particle refinement has been applied by grinding as well as ball milling. For the ternary alloys a uniform distribution was observed with secondary electron microscopy, which was attributed to the lower melting point of DyNdCu and TbNdCu compared to DyCu. Additional annealing at 600°C leads to a diffusion of Dy or Tb into the Nd-Fe-B flakes, which was observed by transmission electron microscopy. This diffusion modifies the grain boundary phase and thus further enhances coercivity without decreasing remanence. The highest coercivity was observed for TbNdCu. Following this, hot-compacted magnets have been die-upset in order to prepare textured magnets. [1] Park et al. Proc. 16th REPM (Sendai, Japan) (2000) p.257

MA 24.8 Wed 11:30 H 0112

Computational search for rare-earth-free hard-magnetic materials — •Jose A. Flores Livas, S. Sharma, K. Dewhurst, and E. K. U. Gross — Max-Planck-Institut für Mikrostrukturphysik. Weinberg 2, 06120. Halle (Saale) Germany.

It is difficult to overstate the importance of hard magnets for human life in modern times; they enter every walk of our life from medical equipments (NMR) to transport (trains, planes, cars, etc) to electronic appliances (for house hold use to computers). All the known hard magnets in use today contain rare-earth elements, which are expensive and environmentally harmful. Rare-earths are also instrumental in tipping the balance of world economy as most of them are mined in limited specific parts of the world. Hence it would be ideal to have similar characteristics as a hard magnet but without or at least with reduced amount of rare-earths. This is the main goal of our work: search for rare-earth-free magnets.

To do so we employ a combination of cutting edged density-functional theory and advanced methods of crystal structure prediction. In our high-throughput scheme, the quantities that define a hard magnet are magnetic anisotropy energy (MAE) and saturation magnetization (M_s), which are the quantities we maximize in search for an ideal magnet.

In my talk I will present details of the computation search algorithm, the improved descriptor and the determination of anisotropy constants, together with some potential and newly discovered rare-earth free hard magnet.

MA 24.9 Wed 11:45 H 0112

Phase Formation and Hot Compaction of Mn-Ga $L1_0$ Hard Magnets — •Torsten Mix[1,2], Ludwig Schultz[1,2], and Thomas George Woodcock[2] — [1]IFW Dresden, Institute for Metallic Materials, PO Box 270116, 01171 Dresden, Germany — [2]Department of Physics, TU Dresden, Dresden, Germany

The Mn-Ga binary system contains phases with high magnetocrystalline anisotropy, which may be suitable candidates for rare earth free permanent magnets. Depending on the composition, $L1_0$ ($cP4$; $P4/mmm$) or $D0_{22}$ ($tI8$; $I4/mmm$) structured phases can be produced. The aim of this work is to understand the formation and stability of the $L1_0$ phase and to optimise both the intrinsic and extrinsic magnetic properties of the alloys. Mn-Ga binary alloys with compositions in the range 55-65 at.% Mn were produced by arc melting and annealing. Phase formation was studied using thermal analysis, x-ray diffraction and magnetometry. Measurements of the magnetocrystalline anisotropy constant and anisotropy field were performed in applied magnetic fields of 14 T. An improvement in the H_c of the Mn-Ga alloys was obtained by producing powder from bulk $L1_0$ materials by mechanical milling. The $L1_0$ powder had a similar magnetisation but a fivefold higher H_c compared to the bulk sample (cf. $Mn_{60}Ga_{40}$: powder: $H_c = 0.376$ T, bulk: $H_c = 0.073$ T). Partial alignment of the $L1_0$ powder in a magnetic field was possible, giving a possible route to the production of anisotropic magnets. Furthermore, fully dense, isotropic, hot compacts were produced in which the improved magnetic properties of the powders were retained.

MA 24.10 Wed 12:00 H 0112

Coercivity enhancement in HDDR based hot pressed and die-upset magnets by in situ grain boundary diffusion — •Christoph Schwöbel[1], Sandro Szabó[1], Simon Sawatzki[1], and Oliver Gutfleisch[1,2] — [1]TU Darmstadt, Deutschland — [2]Fraunhofer IWKS, Hanau, Deutschland

The hydrogenation, disproportionation, desorption, recombination (HDDR) process is a possibility to create submicron grains from Nd-FeB magnets. Hydrogen absorption at elevated temperatures leads to disproportionation followed by subsequent desorption and the formation of an ultrafine grained microstructure. Grain sizes are then close to the critical single domain size for NdFeB. These fine grained HDDR powders are then consolidated and textured by hot compaction and die-upsetting together with a dysprosium containing low melting compound. The applied heat treatment enables a diffusion of Dy along the grain boundaries. This grain boundary diffusion process (GBDP) leads to a further increase in coercivity.
In this study, different starting powders were treated by the HDDR process and mixed with different amounts of DyCu prior to the consolidation. The influence of the different process routes on magnetic properties and microstructure is investigated. Magnetometry and electron microscopy showed a significant increase in H_c after hot compaction if Dy is added. Die-Upsetting led to an increase in remanence due to texturing.

MA 24.11 Wed 12:15 H 0112

Development of Microstructure in Mn-Al-C Permanent Magnetic Materials — •Florian Bittner[1,2], Ludwig Schultz[1,2], and Thomas George Woodcock[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, 01171 Dresden, Germany — [2]Department of Materials Science, TU Dresden, Dresden, Germany

Mn-Al based materials have the potential for an application as rare earth free permanent magnets and could replace Nd-Fe-B in certain areas where the highest energy density is not required. The metastable τ phase in near equiatomic Mn-Al alloys is $L1_0$ structured and has high saturation magnetisation and magnetocrystalline anisotropy. Carbon atoms on interstitial sites increase the thermal stability of the τ phase, enabling processing at higher temperatures. In order to develop anisotropic magnetic properties, an easy axis texture must be induced by hot working. Coercivity strongly depends on microstructure and the presence of defects in the material is particularly important. In order to optimise the coercivity, it is therefore necessary to have detailed knowledge of the microstructural features which appear in these magnets, especially the type of defects, their formation mechanisms and the effect of processing on their fractions. Mn-Al-C magnets have therefore been studied in the as-cast, annealed and hot worked states using electron backscattered diffraction. Two different twinning systems were found to exist in the as-cast material, the fractions of which changed after hot working. These crystalline defects, other microstructural parameters and the magnetic properties will be discussed in terms of the various processing steps applied.