MA 3: Magnetic Materials for Efficient Energy Conversion

Time: Monday 9:30–12:30 Location: HSZ 401

MA 3.1 Mon 9:30 HSZ 401

Voltage-driven giant modulation of magnetism in ferro- and ferri-magnetic alloys — •Xinglong Ye[1,2], Harish Singh[1], Hongbin Zhang[1], Holger Gesswein[3], Reda Chellali[2], Ralf Witte[2], Alan Molinari[2], Konstantin Skokov[1], Oliver Gutfleisch[1], Horst Hahn[2], and Robert Kruk[2] — [1]Department of Material Science, Technical University Darmstadt — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology — [3]Institute of Applied Materials, Karlsruhe Institute of Technology

Controlling magnetism and magnetic properties by small voltages have become one of the core research topics vigorously pursued in magnetoelectric actuation, spintronics and data storage. In magnetically-ordered metals and alloys, however, the voltage effect is usually limited to the scale of atomic layers due to strong electric-field screening. Here, we propose to control their magnetism and magnetic properties by electrochemically-driven insertion/extraction of hydrogen atoms in interstitial sites. Using this approach, we have tuned the magnetocrystalline anisotropy and coercivity of SmCo5 with micrometer-sized particles by more than 1 T by applying voltages as low as 1 V. Consequently, a voltage-assisted and -controlled magnetization reversal has been achieved at room temperature for the first time in permanent magnets. Furthermore, we will show that our electrochemically-driven hydrogen charging can switch the perpendicular anisotropy to in-plane anisotropy in ferrimagnetic thin films with high anisotropy energy, which further exemplifies the universality of our approach in controlling magnetism of rare earth - containing materials.

MA 3.2 Mon 9:45 HSZ 401

Additive Manufacturing of (Pr,Nd)-Fe-Cu-B Permanent Magnets — •Jianing Liu[1], Ruiwen Xie[2], Alex Aubert[1], Lukas Schäfer[1], Holger Merschroth[3], Jana Harbig[3], Ying Yang[4], Philipp Gabriel[4], Anna Ziefuss[4], Stefan Barcikowski[4], Matthias Weigold[3], Hongbin Zhang[2], Oliver Gutfleisch[1], and Konstantin Skokov[1] — [1]Functional Materials, Technical University of Darmstadt — [2]Theory of Magnetic Materials, Technical University of Darmstadt — [3]Institute of Production Management, Technology and Machine Tools, Technical University of Darmstadt — [4]Technical Chemistry I, University of Duisburg-Essen

Additive Manufacturing (AM) of permanent magnets is a new and challenging field in material science and engineering. To obtain a microstructure necessary for high coercivity is by no means straightforward, especially after fast cooling in Laser Powder Bed Fusion (L-PBF). In order to achieve the desired microstructure and hard magnetic properties, we propose the Pr-Fe-Cu-B as a new useful reference alloy system and compare with its Nd-based counterpart. Our studies describe the L-PBF and the subsequent annealing optimization in order to understand the newly established coercivity mechanism. Specifically, we explore the 6-13-1-type grain boundary phase and grow single crystals to understand its magnetism, supported by DFT calculations. Furthermore, grain boundary engineering with nanoparticles shows great potential on grain refinement and uniaxial grain growth during re-solidification during L-PBF. We acknowledge the support of the Collaborative Research Centre/Transregio 270 HoMMage.

MA 3.3 Mon 10:00 HSZ 401

Simultaneous measurements of X-ray absorption, diffraction and bulk properties in $HoCo_2$ — •Katharina Ollefs[1], Gabriel Gomez-Eslava[1], Alex Aubert[2], Konstantin Skokov[2], Alexey Karpenkov[2], Oliver Gutfleisch[2], Fabrice Wilhelm[3], Andrei Rogalev[3], Damian Günzing[1], Johanna Lill[1], Benedikt Eggert[1], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Functional Materials, Technical University Darmstadt, Germany — [3]European Synchrotron Radiation Facility, France

Bulk properties and atomistic/local parameters determined by X-ray Absorption Spectroscopy (XAS) or scattering are typically measured on different samples (such as powder) with the same composition. Together with the influence of the different sample environments in different setups this prevents a direct correlation of microscopic and macroscopic observations, especially for materials exhibiting dramatic changes of their properties around phase transitions. Here we present the ULMAG [1] set up. To demonstrate the capability of our technique we measured, a polycrystalline $HoCo_2$ sample. We show the magnetic field dependence of X-ray Magnetic Circular Dichroism (XMCD), stray field, longitudinal and transversal strain and sample temperature. Furthermore we demonstrate the capability to measure XAS/XMCD and diffraction on a single grain inside this material. [1] Aubert, Alex, et al. IEEE Transactions on Instrumentation and Measurement 71 (2022): 1-9. Supported by the DFG CRC TRR 270 HoMMage, the BMBF project ULMAG and the ESRF by beamtime allocation.

MA 3.4 Mon 10:15 HSZ 401

A thorough TEM investigation of B2 ordered FeRh (50/50) alloy — •Esmaeil Adabifiroozjaei[1], Nagaarjhuna Kani[1,2], Robert Winkler[1], Tianshu Jiang[1], Oscar Recalde[1], Alexander Zintler[1], Alisa Chirkova[2], Konstantin Skokov[2], Oliver Gutfleisch[2], and Leopoldo Molina Luna[1] — [1]Advanced Electron Microscopy, Department of Materials- and Earth Sciences, Technical University of Darmstadt, Germany — [2]Functional Materials, Department of Materials- and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany

Fe50Rh50 alloys are known to have a B2 structure with an antiferromagnetic to ferromagnetic transition at near room temperature. Since this alloy can be considered as betta alloy (CdAu, TiNi, Fe-C, etc), it is expected to present a pre-martensite structure followed by a martensite structure upon cooling at cryogenic temperature. The martensite was also predicted by extensive first principal calculations. However, so far, no evidence has been given regarding the formation of either pre-martensite or martensite structures in the Fe50Rh50 alloy. Here, we use various TEM techniques (including CTEM, HRTEM, STEM (HAADF), and EDS) to investigate the FeRh 50/50 alloy and demonstrate that although the structure of the alloy matches the B2 BCC structure, there is systematic modulation along certain reflexes (100 and 110). We believe that the existence of such ordered modulation along certain directions are indicative of a pre-martensite structure.

MA 3.5 Mon 10:30 HSZ 401

Shaping and functionalizing of Gd for a magnetocaloric cooling application — •Lukas Beyer[1,2], Bruno Weise[1], Julia Kristin Hufenbach[1,2], and Jens Freudenberger[1,2] — [1]Leibniz IFW Dresden, Institute for Complex Materials, Helmholtzstr. 20, 01069, Dresden, Germany — [2]TU Bergakademie Freiberg, Institute of Materials Science, Gustav-Zeuner-Str. 5, 09599, Freiberg, Germany

Magnetic refrigeration based on the magnetocaloric effect aims to substitute conventional cooling solutions, still, shaping and use of magnetocaloric materials remains challenging [1]. A combination with so-called thermal switches could improve the heat transport resulting in higher operating frequencies and therefore, an increase in the power density of magnetic cooling [2]. This could be beneficial for battery thermal management systems [3]. In this work we studied the influence of mechanical deformation on Gd while producing Gd-substrates that could be combined with fast thermal switches by ElectroWetting On Dielectric. We prepared Gd-substrates via cold-rolling and strip casting and investigated these in regards of sufficient surface quality and substrate dimensions. Heat treatments have been performed to restore the magnetocaloric effect after deformation. By means of magnetic and heat-capacity measurements we calculated the isothermal entropy and adiabatic temperature change and proved the recovery of the magnetocaloric effect in Gd-substrates. [1] J. S. Brown, et al.;Appl. Therm. Eng. 64 (2014). [2] A. Kitanovski, et al.;Int.J. Refrig. 33 (2010). [3] J. Kim et al.;Appl. Therm. Eng. 149 (2019).

MA 3.6 Mon 10:45 HSZ 401

Large Room Temperature Anomalous Transverse Thermoelectric Effect in Kagome Antiferromagnet YMn6Sn6 — •Subhajit Roychowdhury[1], Andrew M. Ochs[2], Satya N. Guin[1], Kartik Samanta[1], Jonathan Noky[1], Chandra Shekhar[1], Maia G. Vergniory[1], Joshua E. Goldberger[2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]The Ohio State University, Columbus, 43210 Ohio, United States

Kagome magnets possess several novel non-trivial topological features owing to the strong correlation between topology and magnetism, that extends to their applications in the field of thermoelectricity. Conventional thermoelectric (TE) devices use the Seebeck effect to convert heat into electrical energy. In contrast, transverse thermoelectric devices based on the Nernst effect are attracting recent attention due to their unique transverse geometry, which uses a single material to eliminate the need for a multitude of electrical connections compared to conventional TE devices. In this study, we obtain a large anomalous transverse thermoelectric effect of ~ 2 microV K-1 at room temperature in a kagome antiferromagnet YMn6Sn6 single crystal. The obtained value is larger than that of state-of-the-art canted antiferromagnetic (AFM) materials and comparable with ferromagnetic systems. The large anomalous Nernst effect (ANE) can be attributed to the net Berry curvature near the Fermi level.

15 min. break

MA 3.7 Mon 11:15 HSZ 401

Tailoring of thermal hysteresis in Ni-Mn-Sn shape memory alloys via microstructure design — •Franziska Scheibel[1], Chistian Lauhoff[2], Johannes Puy[1], David Koch[1], Philipp Krooss[2], Thomas Niendorf[2], and Oliver Gutfleisch[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany — [2]Universität Kassel, Kassel, Germany

Ferromagnetic shape memory alloys (FSMA) like Ni-Mn-Sn undergo a magneto-structural transition and show giant multicaloric properties. Thus, these materials are excellent for caloric refrigeration as an energy efficient, environmentally friendly and safe alternative for vapor compression cooling. However, tailoring of the inherent thermal hysteresis is essential for material development [1].

The hysteresis can be influenced by the microstructure (grain configuration and size, texture, defects, or internal stress) [2]. In this study, the grain size and arrangement have been modified by powder-based processing using spark-plasma sintering and additive manufacturing technique to tailor both the microstructure and the thermal hysteresis at the same time. The understanding of the relation between grain-size, texture, grain arrangement and multiple external stimuli is essential to develop materials with first-order magneto-structural transition transformation for multicaloric cooling.

This work was supported by the ERC Advanced Grant "Cool Innov" and the SFB-TRR270 "HoMMage".

[1] F. Scheibel et al., Energy Technol. 6, 1397 (2018)
[2] O. Gutfleisch et al., Phil. Trans. R. Soc. A 374: 20150308 (2016)

MA 3.8 Mon 11:30 HSZ 401

Impact of disorder on the vibrational and magnetic properties of Ni-Mn-(Sn,In) Heusler alloys — •Olga N. Miroshkina[1], Benedikt Eggert[1], Johanna Lill[1], Benedikt Beckmann[2], David Koch[2], Katharina Ollefs[1], Francesco Cugini[3], Massimo Solzi[3], Mojmir Šob[4], Martin Friák[4], Oliver Gutfleisch[2], Heiko Wende[1], and Markus E. Gruner[1] — [1]University of Duisburg-Essen, Duisburg, Germany — [2]Technical University of Darmstadt, Darmstadt, Germany — [3]University of Parma, Parma, Italy — [4]Czech Academy of Sciences, Brno, Czech Republic

Ni-Mn-Z with Z=In,Sn Heuslers are promising magnetocaloric systems to be employed in the magnetic cooling devices. In this respect, it is important to understand the influence of the main group element on the vibrational and magnetic properties of these materials. By combining large-scale density functional theory calculations with ^{119}Sn-NRIXS and Mössbauer spectroscopy, we disentangled the vibrational contributions of the Sn atoms in Ni_2MnSn. We found the evidence that inversion of optical modes at Γ involving the displacement of Ni and the heavier Z atoms predicted previously for other Ni-Mn-based Heuslers is also a property of Ni_2MnSn, while deviation between experimental spectra and simulations might be explained by site-disorder [1]. In turn, the variation of Z in combination with chemical disorder can be employed to control the magnetization of the transition metal sublattice [2]. This work is funded by DFG within CRC/TRR 270.

[1] O.N. Miroshkina, B. Eggert *et al.*, PRB (accepted) (2022).
[2] F. Cugini *et al.*, PRB 105, 174434 (2022).

MA 3.9 Mon 11:45 HSZ 401

Tailoring thermal hysteresis and microstructure of Ni-Mn-based Heusler alloys for multicaloric cooling applications — •Andreas Taubel[1], Franziska Scheibel[1], Lukas Pfeuffer[1], Benedikt Beckmann[1], Navid Shayanfar[1], Tino Gottschall[2], Konstantin Skokov[1], and Oliver Gutfleisch[1] — [1]TUDarmstadt, Material Science, 64287 Darmstadt — [2]Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR, 01328 Dresden

Refrigeration based on the magnetocaloric effect (MCE) attracts a lot of attention since it can be more energy efficient and environmentally friendly than current vapor compression technology. The concept uses a solid-state magnetic material that heats up and cools down cyclically when exposed to a changing magnetic field. The problem of thermal hysteresis for efficient materials with a first-order phase transition can be overcome by applying stress as a second stimulus [1].

In this work, we develop Ni-Co-Mn-In and Ni-Co-Mn-Ti Heusler alloys towards using them in a novel multi-stimuli cooling concept. We investigated the influence of different microstructures from chemical variation and different processing routes on the magnetocaloric and elastocaloric performance of these materials [2,3]. The introduction of secondary phases significantly enhances the mechanical stability.

We acknowledge funding by ERC (Adv. Grant Cool Innov, GrantNo. 743116) and by DFG (CRC HoMMage, ID 405553726 *TRR 270)

[1] T. Gottschall et al., Nature Mat. 17, 929*934 (2018)
[2] L. Pfeuffer et al., Acta Materialia 217 1175157 (2021)
[3] A. Taubel et al., Acta Mater. 201, 425-434 (2020)

MA 3.10 Mon 12:00 HSZ 401

Influence of Cu addition and chemical order on the thermomagnetic properties of Ni-Mn-Ga-based films — •Lukas Fink[1,2,3], Kornelius Nielsch[2,3], and Sebastian Fähler[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, D-01328 Dresden, Germany — [2]Leibniz IFW Dresden, Institute for Metallic Materials, D-01171 Dresden, Germany — [3]TU Dresden, Institute of Materials Science, D-01062 Dresden, Germany

One way to harvest low-grade waste heat is a microscale thermomagnetic generator (TMG), which uses magnetocaloric films as active material. The high surface-to-volume ratio of thin films enables a fast heat transfer, increasing the cycling frequency and power density compared to bulk devices. Selecting the optimal active material is decisive for the efficiency of a TMG since it will determine the temperature regime and the cycling frequency. Recently Ni-Mn-based Heusler alloys were proposed as they can be prepared by standard thin-film technologies.

Here we use combinatorial growth of Cu alloyed Ni-Mn-Ga films and subsequent heat treatment for systematic optimization of thermomagnetic properties. We examine the key thermomagnetic properties like 1) the working temperature T^* and 2) the performance $\frac{\Delta M}{\Delta T}$ and correlate them with common properties like 3) crystal structure, 4) 1st and 2nd order transition and 5) spontaneous magnetization. Within our research, we can disentangle the effects of valence electron number e/a and chemical order. This work is funded by the DFG (FA453/14).

MA 3.11 Mon 12:15 HSZ 401

Study of the corrosion behaviour of Ni-Co-Mn-In Heusler — •Ulysse Rocabert, Lukas Pfeuffer, and Oliver Gutfleisch — Functional Materials Group, Department of Materials and Earth Sciences, Technische Universität Darmstadt, Alarich-Weiss-Straße 16, 64287 Darmstadt, Germany

Heusler materials are one of the promising material classes that are considered for their very useful magnetocaloric properties at room temperature. While their magnetic and mechanical properties have seen broad investigation, their electrochemical properties especially in aqueous environment remain largely unstudied. This study focuses on the characterization of such properties of Ni-Co-Mn-In alloys in different chemical environments and proposes a assessment on their implementation into refrigeration systems in comparison with LaFeSi-Mn alloys.