MA 11: Focus Session: Magnetic materials for energy efficient applications

Time: Monday 15:45–18:45 Location: H38

Invited Talk MA 11.1 Mon 15:45 H38

Microstructure optimization for rare-earth efficient permanent magnets — •Thomas Schrefl[1], Johann Fischbacher[1], Alexander Kovacs[1], Lukas Exl[2], Kazuya Yokota[1,3], and Tetsuya Shoji[3] — [1]Danube University Krems, Austria — [2]Wolfgang Pauli Institute, c/o University of Vienna, Austria — [3]Toyota Motor Corporation, Japan

Permanent magnets are widely used in modern society including consumer electronics, transport, and power generation. The key figures of merit, coercive field and energy density product, depend on the interplay between the intrinsic magnetic properties and the microstructure. We use synthetically generated grain structures to model the influence of grain morphology and grain boundary phases on coercivity. By computing the lowest saddle point for magnetization switching we find the weakest point in the structure, where magnetization reversal starts. We apply machine learning to quantify the reduction of coercivity caused by different microstructural features. Again, regions where the local coercive field is much lower than the average can be identified. Our results suggest that adding heavy rare-earth elements through grain boundary diffusion to these specific regions only will be sufficient to increase coercivity. Thus, the magnet's performance and temperature stability may be improved with a minimum amount of heavy rare-earth elements. Examples will be given for $Nd_2Fe_{14}B$ and $SmFe_{11}Ti$ based magnets.

Work supported by Toyota Motor Corporation and the Austrian Science Fund (grant no F41, P31140).

Invited Talk MA 11.2 Mon 16:15 H38

Advanced methods for the development of high performance hard and soft magnetic materials — •Dagmar Goll and Gerhard Schneider — Aalen University, Materials Research Institute, Beethovenstr. 1, 73430 Aalen, Germany

Higher efficiency in electro mobility requires high performance and economic motor concepts. Recent progresses in the development of hard and soft magnetic materials and their production processes offer new possibilities to further improve electric energy converters. For permanent magnets remaining challenges are the dependence on critical rare earth elements and the limited possibility to optimize the microstructure to approach theoretical predictions of micromagnetism. Equally important is the minimization of magnetic losses in soft magnetic cores. Innovative synthesis processes like high-throughput experiments and additive manufacturing by laser powder bed fusion offer new degrees of flexibility. These allow optimized alloy compositions and microstructures as well as novel topological structures and multilayer composites. Selected examples for different hard and soft magnetic prototypes and their performance will be presented.

MA 11.3 Mon 16:45 H38

Microscopic insights into the disorder induced phase transition in FeRh thin films — •Benedikt Eggert[1], Alexander Schmeink[2,3], Kay Potzger[2], Jürgen Lindner[2], Jürgen Fassbender[2,3], Katharina Ollefs[1], Werner Keune[1], Rantej Bali[2], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]Dresden University of Technology, Germany

By employing ^{57}Fe conversion electron Mössbauer spectroscopy, we qualitatively determined the changes of the microscopic Fe moment of chemical disordered epitaxial B2-FeRh(001) thin films, where the chemical disorder has been induced by ion irradiation with Ne^+. Apart from the initial magnetic splitting at 25.4 T an additional sextet contribution arises with an hyperfine field of 27.4 T. A comparison between the structural disorder and the temperature induced phase transition shows a similar change of the ^{57}Fe hyperfine field as a function of the macroscopic magnetisation. This gives an indirect indication, that the metamagnetic phase transition proceeds via a defect-driven domain nucleation of ferromagnetic domains in the antiferromagnetic matrix, as it was suggested based on XPEEM and nano-XRD measurements along the phase transition [1]. We would like to thank the Ion Beam Center at Helmholtz-Zentrum Dresden-Rossendorf for providing the necessary facilities and acknowledge the financial support by DFG (WE2623/17-1).

[1] D. Keavney et al. Scientific Reports 8 1778 (2018)

15 min. break

Invited Talk MA 11.4 Mon 17:15 H38

Compositionally graded films as model systems to study magnetic materials for energy applications — •Nora Dempsey — Univ. Grenoble Alpes, CNRS/UGA, Grenoble INP, Institut Néel, Grenoble, France

Combinatorial thin film studies are being used for the screening and optimization of a range of functional materials [1]. The basic idea is to produce compositionally graded films, to allow high throughput screening of materials properties as a function of composition, as well as other processing parameters such as deposition temperature and post-deposition annealing. In this talk I will present studies of compositionally graded films of two types of magnetic materials of interest for energy applications, namely hard magnetic materials and magnetocaloric materials. Films were produced by sputtering asymmetric targets. Composition variations were characterised using EDX mapping while structural and magnetic characterisation was performed with SEM, XRD and magnetometry. A scanning polar MOKE set-up incorporating a bipolar pulsed magnetic field system capable of applying fields of up to 10 T was specifically developed for high throughput magnetic characterisation of these compositionally graded films [2]. The relationship between processing parameters and structural and magnetic properties will be presented.

[1] M. L. Green, I. Takeuchi, and J. Hattrick-Simpers, J. Appl. Phys. 113 (2013) 231101 [2] A. Dias, Gabriel Gomez, Dominique Givord, et al., AIP ADVANCES 7 (2017) 056227

Invited Talk MA 11.5 Mon 17:45 H38

Dissecting the magneto-structural transformation in materials with first-order field-induced transitions — •Konstantin Skokov — Technische Universität Darmstadt, 64287 Darmstadt, Germany

We report on a detailed study of the evolution occurring in the magnetic, electronic and structural subsystems of FeRh, La(FeSi)13, MnAs and Heuslers alloys, when the materials pass through a first-order field-induced transition. We have built a unique experimental setup which allows us to investigate the correlation between changes occurring in magnetization, magnetostriction, resistivity and the resulting magnetocaloric effect (MCE). The field-induced transitions from antiferromagnetic/paramagnetic to ferromagnetic states do not complete in one single step, as is commonly assumed. In fact, there are some well-distinguished and system dependent stages of the transition. In some stages the increase of magnetization and resulting MCE is the consequence of transformations taking place mainly in electronic subsystems containing carrying magnetic moment itinerant 3d electrons. In other stages the transformation in the electronic and magnetic subsystems is the result of lattice expansion/contraction. We demonstrate that it is possible to lock the sample in the intermediate state when the lattice parameters relate to the antiferromagnetic/paramagnetic state and the electronic structure and magnetization relate to the ferromagnetic state.

The work was supported by funding from the European Research Council (ERC), grant no. 743116 - project Cool Innov

MA 11.6 Mon 18:15 H38

Design of control field pulses to efficiently induce magnetic transitions — •Pavel F. Bessarab[1,2] and Grzegorz Kwiatkowski[1,3] — [1]University of Iceland, Reykjavík, Iceland — [2]ITMO University, St. Petersburg, Russia — [3]Immanuel Kant Baltic Federal Uni- versity, Kaliningrad, Russia

Control of magnetization switching is of critical importance for the development of novel, energy efficient magnetic memory devices. Transitions between stable magnetic states can follow various pathways which are not equivalent in terms of efficiency and required time. In this study, we propose a general theoretical approach to design external field pulses for efficient switching between magnetic states. The approach involves calculation of a minimum energy path (MEP) for desired magnetic transition and systematic identification of the temporal and spatial shape of the pulse needed to drive the system along the MEP.

The approach is applied to the magnetization switching in the atomically-thin Fe nanowires on Cu_2N surface, a system that has previously been studied extensively in the laboratory [1]. Short nanowires reverse their magnetization via coherent rotation which is induced by applying a uniform magnetic field. Transitions in longer chains involve nucleation and propagation of transient domain walls, for which a localized, time-dependent pulse needs to be applied. Our results demonstrate that efficient switching pulses can be predicted from first principles, contributing to the development of low-power technologies.

[1] A. Spinelli et al., Nature Mater. **13**, 782 (2014).

MA 11.7 Mon 18:30 H38

Computational Design of Heusler Alloys for Energy Applications — •Nuno M. Fortunato, Qiang Gao, Ingo Opahle, Oliver Guttfleisch, and Hongbin Zhang — Institute of Materials, TU Darmstadt, Darmstadt, Germany

Heusler alloys are multi-functional materials with a wide range of potential applications, among them permanent magnets and magnetic refrigeration, which are relevant for energy efficient industrial and commercial processes.

A great deal of experimental effort has been put into exploiting the Heusler family's large number of possible compositions and substitutional disorder. To accelerate this search we perform a high-throughput Density Functional Theory screening of material properties of stochiometric all-d-metal based Heuslers and MM'X (M=metal, X= main group) hexagonal/orthorhombic compounds [2], looking at the stability of the martensite and austenite phases.

Further, permanent magnet relevant properties like tetragonality, magnetic anisotropy energy, saturation magnetization and Curie temperature are calculated. We found 192 stable all-d-metal Heusler alloys where the martensite is the lower energy phase, of which 44 are also stable in the austenite. To elucidate the feasibility of these compounds as magnetocaloric materials we look at the Bain path, magneto-volume coupling [2], mechanical stability and interplay of magnetic and structural transition temperatures estimates.

[1] . A. Taubel et al., J. Phys. D: Appl. Phys **51**, 464005 (2017);
[2] . J.D. Bocarsly, et al., Chem. Mater. **29**, 1613 (2017);