MA 7: Bulk Magnetic Materials and Magnetic Particles/Clusters

Time: Monday 9:30–12:45 Location: EB 407

MA 7.1 Mon 9:30 EB 407

Theoretical Investigation of the Effect of Si and Co Doping on the Physical and Magnetic Properties of Rare-Earth-Free Fe_2P Magnets — •Stephan Erdmann, Halil Ibrahim Sözen, and Thorsten Klüner — Carl von Ossietzky University Oldenburg

Due to the resource criticality of rare-earth (RE) elements, there is a great interest in finding a RE-free magnet to fill in the gap between the commonly used ferrites and the $Nd_2Fe_{14}B$ magnets. A potential candidate to fill in this gap are magnets based on the Fe_2P compound, which exhibits a high magnetisation and high uniaxial anisotropy. In this work, we have performed density functional theory calculations to investigate the influence of the substitution of P and Fe by readily available elements such as Si and Co on the magnetic and physical properties of the Fe_2P compound. Both elements have been chosen because they are known to increase the Curie temperature of Fe_2P. For a systematic understanding, properties such as the formation energy at 0 K, as well as magnetic properties like the magnetization M_S and the Curie temperature T_C are screened starting from the binary structure of Fe_2P. Furthermore, the combined effects of Si and Co substitution on the physical and magnetic properties are considered in quarternary $(Fe,Co)_2(P,Si)$ compounds. The T_C trends of these quarternary compounds were investigated by the calculation of exchange interaction energies J_{ij}, which revealed a positive influence of Si on the 3f-3g Fe interactions leading to an increase in T_C. Co substitution leads either to an increase or decrease of the 3f-3f and 3g-3g Fe interactions and thus on T_C for low and high Si contents, respectively.

MA 7.2 Mon 9:45 EB 407

A magnetic C36 Laves phase in Co-Fe-Ta system — •Sergiu Arapan[1], Pablo Nieves[2], Jakub Šebesta[3], Andrea Dzubinska[4], Marian Reiffers[5], and Dominik Legut[1] — [1]VŠB - Technical University of Ostrava, Czech Republic — [2]University of Oviedo, Spain — [3]Uppsala University, Sweden — [4]University Pavol Jozef Safarik, Košice, Slovakia — [5]University of Prešov, Slovakia

Modern computational tools that use a combination of electronic structure calculations, adaptive genetic algorithms, and machine learning data analysis, allow for an unprecedented prediction of new structures with desired physical properties. Yet, in many cases, no recipes are provided to synthesize them. In the case of a binary compound, we show a route to bring a theoretically predicted structure to a real material. In particular, we demonstrated the possibility to synthesize a C36 Laves phase (hP24 structure) with improved intrinsic magnetic properties in the Co-Fe-Ta system. Computational studies predict superior intrinsic magnetic properties for an experimentally not observed Fe_2Ta C36 Laves phase. This phase, however, occur in the Co-Ta system, which suggests the possibility of the existence of a stable compound along the $(Co_{1-x}Fe_x)_2Ta$ path. Following this route, we computationally predict a stable C36 Laves phase with improved intrinsic magnetic properties for large Fe content, and successfully synthesize it experimentally. This approach is general and can be applied to identify a synthesis path for a predicted material with desired properties.

MA 7.3 Mon 10:00 EB 407

Data-Mining Search for Rare-Earth-Free Permanent Magnets Among Predicted Crystal Structures — •Alena Vishina, Olle Eriksson, and Heike C. Herper — Department of Physics and Astronomy, Uppsala University, Sweden

Magnetic materials for energy applications (e.g. electric motors and wind turbines) is a boosting area of research, as many compounds used nowadays are based on undesirable expensive and environmentally-challenging rare earth (RE) elements. At the same time, with the increasing power of supercomputers and recent developments in machine-learning, new stable and metastable materials are being predicted that have never been synthesized before. The databases of such materials are an open field for data-mining searches for specific material properties.

One of the aforementioned databases [1] was used as an input for our recent investigation [2]. Filtering through around a million of compounds, we were searching for stable and meta-stable (likely to be synthesizable) materials with high magnetization, large uniaxial magnetocrystalline anisotropy, and high Curie temperature. The promising candidates were also tested for dynamic stability. Four systems were found that should be further explored as the candidates novel RE-free PMs - Ta3ZnFe8, AlFe2, Co3Ni2, and Fe3Ge.

Ref. 1. J. Schmidt et al, Materials Cloud archive 2022.126 (2022) 2. A. Vishina et al, Acta Materialia, 261, 119348 (2023)

MA 7.4 Mon 10:15 EB 407

Nano-composites for high performance Nd-Fe-B permanent magnets — •Lukas Schäfer[1], Imants Dirba[1], Fernando Maccari[1], Konstantin Skokov[1], Esmaeil Adabifiroozjaei[2], Leopoldo Molina-Luna[2], and Oliver Gutfleisch[1] — [1]Functional Materials, Materials Science, TU Darmstadt, Darmstadt, Germany — [2]Advanced Electron Microscopy, Materials Science, TU Darmstadt, Darmstadt, Germany

Permanent magnets (PM) based on Nd-Fe-B are important for modern electric motor and generator applications crucial to energy conversion. Especially due to the clean energy transition, which results in a higher demand for electric cars and wind turbines, the need for high performance PM is expected to drastically increase in the coming years. In order to improve the magnetic performance and, at the same time, reduce the content of critical rare earth, the design of nanocomposite microstructures consisting of the hard magnetic and soft magnetic phases is a promising approach. Textured "exchange-spring magnets" could, in theory, surpass the theoretical limit of today s commercial Nd-Fe-B magnets, yet despite three decades of research, bulk, textured nanocomposites with enhanced performance have not been realized yet. In this talk, a novel top-down approach based on the formation of a metastable phase in the Nd-Fe-B system by rapid solidification is presented. Microstructural and magnetic investigations will demonstrate the unique thermal decomposition of this phase into the hard magnetic $Nd_2Fe_{14}B$ phase and soft magnetic nano-precipitates of α-Fe, leading to an enhancement of the remanence.

MA 7.5 Mon 10:30 EB 407

Strong and ductile high temperature soft magnets through Widmanstätten precipitates — •Liuliu Han[1], Dierk Raabe[1], Oliver Gutfleisch[2], Fernando Maccari[2], Ivan Soldatov[3], and Rudolf Schäfer[3] — [1]Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Department of Material Science, Technical University of Darmstadt, 64287 Darmstadt, Germany — [3]IFW Dresden, Institute for Metallic Materials, Helmholtzstr. 20, 01069 Dresden, Germany

Fast growth of sustainable energy production requires massive electrification of transport, industry and households, with electrical motors as key components. These need soft magnets with high saturation magnetization, mechanical strength, and thermal stability to operate efficiently and safely. Reconciling these properties in one material is challenging because thermally-stable microstructures for strength increase conflict with magnetic performance. Here, we present a material concept that combines thermal stability, soft magnetic response, and high mechanical strength. The strong and ductile soft ferromagnet is realized as a multicomponent alloy in which precipitates with a large aspect ratio form a Widmanstätten pattern. The material shows excellent magnetic and mechanical properties at high temperatures while the reference alloy with identical composition devoid of precipitates significantly loses its magnetization and strength at identical temperatures. The work provides a new avenue to develop soft magnets for high-temperature applications, enabling efficient use of sustainable electrical energy under harsh operating conditions.

MA 7.6 Mon 10:45 EB 407

Shape-dependent magnetic study of hematite nanospindles — •Juri Kopp[1], Joachim Landers[1], Soma Salamon[1], Gerald Richwien[2], Benoît Rhein[2], Annette Schmidt[2], and Heiko Wende[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — [2]Institute for Physical Chemistry, University of Cologne

Hematite nanospindles can be synthesized relatively easily in various aspect ratios and can be incorporated in aqueous solutions. When considering hematite-based ferrofluids, the question arises to what extent the degree of particle elongation influences the orientation behavior and mobility of nanospindles. For this purpose, hematite nanospindles with different aspect ratios in a 70 wt% glycerol-water mixture were investigated by magnetic field dependent Mössbauer spectroscopy, as well as magnetometry. As expected, the field-dependent Mössbauer experiments showed that the more elongated particles (aspect ratio of 3.7 and 5.2) were easier to align in the field due to the greater magnetic moment compared to the sample with a ratio of 2.5. Surprisingly the reference powder measurements for the sample with the aspect ratio of 1.0 showed a relatively sharp Morin-transition, in contrast to the rest of the other samples of higher aspect ratio, where no such transition occurred over the entire temperature range. Based on these results, we aim for the incorporation of the nanospindles into liquid crystalline matrices and to investigate anisotropic diffusion in ferronematic phases. We gratefully acknowledge funding by the DFG through LA5175/1-1.

15 min. break

MA 7.7 Mon 11:15 EB 407

Simulation of Interaction and Self-assembly of Magnetically Decorated Particles — •Maximilian Neumann, Sibylle Gemming, Oliver G. Schmidt, Daniil Karnaushenko, and Aaron Steinhäusser — TU Chemnitz, Chemnitz, Germany

The self-assembly of particles of modest complexity into elaborate structures is a governing principle in nature. In particular magnetic particles allow for a highly tunable interaction between them combined with manipulation through external sources (e.g. magnetic fields). By decorating cylindrical particles with permanent magnets in specific patterns along their edges we create distinct species of particles. These magnets are facing perpendicular to the base either in or out of the surface, resulting in a mix of attractive and repulsive interactions between individual magnets of different particles depending on proximity. In this way we facilitate the framework for self-assembly while introducing selectivity between species and different particle arrangements. We show different simulations of assembly schemes with a focus on finding parameters and pattern-groups that create strong attraction and high selectivity for matching patterns and set relative orientation while minimizing interaction across pairs.

MA 7.8 Mon 11:30 EB 407

Controlled transport of 3D anisotropic brick-shaped particles using dynamic magnetic field landscapes for Lab-on-Chip (LOC) applications — •Jonas Bugase, Christian Janzen, Arne Vereijken, Rico Huhnstock, and Arno Ehresmann — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, 34132 Kassel

The controlled interaction of magnetic colloids amongst themselves and with surfaces in the presence of magnetic fields proves to be a valuable tool for studying and manipulating complex biological systems in microfluidic devices [1]. We present a remote-controlled transport mechanism for 3D elongated bricked-shaped magnetic particles, fabricated using two-photon polymerization (2PP) lithography. These particles are thoroughly characterized in terms of their sizes and magnetic properties. The magnetic moment of the polymer brick particles is fixed along the lateral axis by sputtering a magnetic Exchange Bias (EB) thin film system on its surface. The transport occurs within a periodic stray field landscape, artificially created by opposing domain stripe through ion bombardment induced magnetic patterning (IBMP) [2]. We discuss the influence of particle geometry and size in relation to the periodicity of the underlying domain pattern on the transport behavior. This transport mechanism is promising for the detection of biomolecules in Lab-on-Chip devices [3].

[1] Afsaneh *et al.* (2022), Talanta Open, (5): 100092.
[2] Ehresmann *et al.* (2015), Sensors, (15): 28854.
[3] Lowensohn *et al.* (2020), Langmuir, (36): 7100.

MA 7.9 Mon 11:45 EB 407

Application of white light interferometry for the absolute equilibrium height quantification of magnetic microbeads captured by tailored magnetic stray fields above a topographically flat surface — •Yahya Shubbak[1], André Stelter[2], Nikolai Weidt[1], Marco Künne[2], Rico Huhnstock[1], Peter Lehmann[2], and Arno Ehresmann[1] — [1]Institute of Physics & Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, D-34132 Kassel — [2]Institute of Measurement Technology, University of Kassel, D-34121 Kassel

Precise control of magnetic micro- and nanoparticles (MPs) in microfluidic environments allows for novel investigations in biomolecular analyte detection and interactions [1]. Utilizing static magnetic field landscapes from a magnetically patterned substrate, combined with external magnetic field pulses, facilitates translatory motion control of MPs at the micro-scale [2]. The close-to-substrate motion of MPs is sensitive to liquid-mediated particle-substrate interactions [3]. Monitoring changes in these interactions by measuring the equilibrium height of MPs above the substrate surface offers a promising approach for sensitive analyte detection. As a crucial step, we introduce white light interferometry to quantitatively measure the absolute distance between MPs and the underlying magnetic substrate. [1]Lim et al., *J. Phys. D: Appl. Phys.* **50**, 33002 (2017) [2]Holzinger et al., *Appl. Phys. Lett.* **100**, 153504 (2012) [3]Huhnstock et al., *Sci Rep* **12**, 20890 (2022)

MA 7.10 Mon 12:00 EB 407

Studying the influence of magnetic stripe domain size on the magnetophoretic transport of superparamagnetic beads for their controlled spatial fractionation — •Rico Huhnstock[1], Lukas Paetzold[1], Piotr Kuświk[2], and Arno Ehresmann[1] — [1]Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel — [2]Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, Poznań 60-179, Poland

Directed transport of magnetic particles for Lab-on-a-chip applications can be realized by superposing periodic magnetic stray field landscapes, emerging from tailored magnetic domain patterns, with external time-dependent magnetic fields [1]. A transition from a linear (phase-locked) to a non-linear (phase-slipping) motion behavior is typically observed for a critical frequency of the external field [2]. This critical frequency is a function of particle and domain pattern characteristics. Studying the latter influence is the scope of this work: We fabricated magnetic stripe domains of gradually increasing width within the same substrate and explored the motion dynamics of laterally transported superparamagnetic beads on top using an optical microscope. As a result, we observed position-dependent critical frequencies, which we will highlight to be beneficial for the spatial fractionation of beads with different magnetophoretic mobilities.

[1] Holzinger *et al.* (2015), ACS Nano, 9(7):7323.
[2] Yellen *et al.* (2007), Lab on a Chip, 7(12):1681.

MA 7.11 Mon 12:15 EB 407

Dynamic magnetic responses inside Magnetite nanoparticle chains detected by Scanning Transmission X-Ray Microscopy Ferromagnetic Resonance — Thomas Feggeler[1,2], Johanna Lill[1], Damian Günzing[1], Ralf Meckenstock[1], Detlef Spoddig[1], Sebastian Wintz[3], Markus Weigand[3], Benjamin Zingsem[1], Heiko Wende[1], Michael Farle[1], Hendrik Ohldag[2], and •Katharina Ollefs[1] — [1]Faculty of Physics and CENIDE, Duisburg, Germany — [2]Advanced Light Source, LBNL, Berkeley, United States of America — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Magnonic excitation of a nanoparticle chain of Magnetite particles (diameter of about 50 nm) embedded in a bacterium Magnetospirillum Magnetotacticum is measured using Scanning Transmission X-Ray Microscopy detected Ferromagnetic Resonance (TR-STXM) [1]. TR-STXM-FMR features the element specific detection of magnetization dynamics with a spatial resolution < 50 nm and a time resolution in the ps regime. A resonant response of the segments of the nanoparticle chain is identified and confirmed by micromagnetic simulations. The manipulation of the external applied magnetic field further allows to selectively excite different segments inside the nanoparticle chains demonstrating the feasibility of magnonic logic devices [2]. We acknowledge funding from DFG via project OL513/1-1, 321560838 and CRC TRR HoMMage.

[1] Th. Feggeler, et al., Phys. Rev. Res. 3, 033036 (2021).
[2] Th. Feggeler et al. New J. Phys. 25 043010 (2023).

MA 7.12 Mon 12:30 EB 407

Frequency mixing magnetic detection for characterization of SPIONs — •Ali Mohammad Pourshahidi, Andreas Offenhäusser, and Hans-Joachim Krause — Institute of Biological Information Processing, Bioelectronics (IBI-3), Forschungszentrum Jülich, Germany

The research on superparamagnetic iron oxide nanoparticles (SPIONs) explores their magnetic properties for bio-sensing and diagnostics. Frequency Mixing Magnetic Detection (FMMD) exploits SPIONs' nonlinear magnetization under dual-frequency magnetic excitation fields (a low-frequency field f_2 and a high-frequency field f_1). As a result, mixing harmonics in form of $f_1 + n \cdot f_2$ are generated that reveal insights into SPION behavior [1]. FMMD has shown significant potential in biosensing for point-of-care monitoring, offering a portable and a handheld solution [2]. Integration of a static offset magnetic field enables the detection of both even and odd harmonics. This enhancement broadens the diagnostic applications to include multiplex detection and characterization of SPION core size [3,4]. These advancements underscore FMMD's role as a tool, for better understanding of magnetic nanoparticle behavior, which is vital for advancing magnetic bio-sensing technologies. This presentation aims to highlight FMMD's applications in multiplex detection and core size analysis of SPIONs.

1. H.-J. Krause et al. JMMM 311(2007) 436 2. S. Achtsnicht et al. PLOS ONE 14 (2019) e0219356 3. A. M. Pourshahidi et al. Sensors 21(2021) 5859 4. A. M. Pourshahidi et al., JMMM 563 (2022) 169969