MM 11: Topical session: Integrated computational materials engineering for design of new materials III

Time: Monday 15:45–18:00 Location: H39

Topical Talk MM 11.1 Mon 15:45 H39

Search for substitutes of magnetic materials containing critical elements by high-throughput screening and multi-scale modeling — •Christian Elsässer, Wolfgang Körner, Georg Krugel, Matous Mrovec, Daniel F. Urban, and Peter Gumbsch — Fraunhofer IWM, Freiburg, Germany

This lecture will discuss how new magnetic materials can be discovered by computational high-throughput-screening and multi-scale-modeling approaches, to substitute established magnets like $Nd_2Fe_{14}B$, which have outstanding functionalities but also constraining criticalities.

A combinatorial high-throughput-screening approach based on density functional theory (DFT) is employed to search for intermetallic phases with crystal structures and chemical compositions, which have good intrinsic ferromagnetic properties but contain no or less amounts of critical rare-earth elements like Nd in $Nd_2Fe_{14}B$.

To develop magnets from promising magnetic phases requires efficient scale-bridging approaches which take into account how the microstructure influences the magnetic behavior. The size of atomistic models can be increased by tight-binding total-energy and bond-order-potential methods, which are based on DFT and capable to describe extended defects like grain boundaries or lattice dislocations.

A route to magnetic multi-domains and poly-crystals is provided by phenomenological approaches like micro-magnetic or phase-field models, which can be parameterized as well using data bases of materials properties obtained from the atomic level. The lecture will close with an outlook in this direction.

MM 11.2 Mon 16:15 H39

Ab initio analysis of the phase stability of Ce-based hard-magnetic materials — •Halil Ibrahim Sözen, Tilmann Hickel, and Jörg Neugebauer — The Max-Planck-Institut für Eisenforschung GmbH Max-Planck-Straße 1, 40237 Düsseldorf

In recent years, the development in electro-mobility, i.e. the progressive replacement of oil-based fuels in the transportation by electric motors, increased the demand of hard magnetic materials, which are composed of rare-earths (RE) and transition metals (TM). Recently, there are attempts to develop alternative hard magnets that lift the dependence on the small number of RE elements. For this purpose, ab initio high-throughput calculations have been performed with the focus on a few selected magnetic parameters. However, the decisive question of the phase stability of potential material systems is much less investigated. For example, for Ce-based alloys the magnetically interesting CeFe11Ti phase is thermodynamically competing with a CeFe2 phase. In order to predict phase stability, we perform ab initio calculations for the Helmholtz free energy F(T,V) taking vibrational, electronic, magnetic and configurational entropy contributions into account. We carefully investigate the performance of density functional theory (DFT) and its extensions to achieve these results and compare the results with Nd-based hard-magnetic materials. Based on these results we provide suggestions as to how the favourable magnetic phases can be stabilized.

MM 11.3 Mon 16:30 H39

Theoretical screening of 1-12 and 1-12-X phases on the search for new hard-magnetic compounds with low rare-earth content — Wolfgang Körner, •Georg Krugel, Daniel F. Urban und Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

The $ThMn_{12}$-type crystal structure recently attracted renewed experimental and theoretical interest as being a promising starting point in the search for new hard-magnetic compounds with low rare-earth content. This is mainly due to the atomic rare-earth to transition-metal ratio of 1:12 and the tetragonal crystal symmetry which is necessary for high magnetocrystalline anisotropy. Estimates of the energy product $(BH)_{max}$ for $NdFe_{12}N$ yield about 686 kJ/m^3 which even exceeds the best available hard magnet nowadays, namely $Nd_2Fe_{14}B$ with $(BH)_{max}$=516 kJ/m^3.

We report on theoretical investigations, by means of density functional theory, of the 1-12 and 1-12-X phases derived from the known $ThMn_{12}$-type structure. We have extended our computational high-throughput screening (HTS) approach [1] by approximate evaluations of the anisotropy constant K_1, the anisotropy field H_a and an estimate of $(BH)_{max}$. Our calculation of K_1 is fast since it is based on the crystal field parameters and avoids expensive total-energy calculations. Besides $NdFe_{12}N$ which has the highest magnetization, several 1-12 and 1-12-X compounds based on Ce instead of Nd are presented which are interesting alternative hard-magnetic compounds.

[1] N. Drebov et al, New J. of Phys. 15, 125023 (2013)

15 min. coffee break

MM 11.4 Mon 17:00 H39

First-principles study of the colour and reflectivity of metals — •Gianluca Prandini[1,2] and Nicola Marzari[1,2] — [1]THEOS, EPF Lausanne, Switzerland — [2]NCCR MARVEL, EPF Lausanne, Switzerland

Gold and copper are the only two elemental metals to show a characteristic colour due to the presence of a drop of the reflectivity curve in the visible range. Reflectivities of all other metals are in general high and flat for all visible frequencies, making they appear shiny and silvery white. Nowadays, with state-of-the-art theoretical methods, it is possible to calculate colour and reflectivity of a material by means of first-principles simulations and, as a practical consequence, predict or design the colour of new alloys. I will show and discuss the results obtained for the reflectivity and colour of elemental metals and of some simple metallic binary alloys. The approach followed for the calculation of the dielectric function is the random-phase approximation (RPA) starting from band structures obtained at the density functional theory (DFT) level using the computationally inexpensive PBE exchange-correlation functional. These results are important in order to establish the computational framework for high-throughput screening of the optical properties of novel metallic alloys.

MM 11.5 Mon 17:15 H39

"Treasure maps" for magnetic CoFeNiCr-based high-entropy-alloys from first-principles — •Fritz Körmann[1], Duancheng Ma[2], Dustin Belyea[3], Matthew Lucas[4], Casey Miller[3], Blazej Grabowski[2], and Marcel Sluiter[1] — [1]Materials Science and Engineering, TU Delft, Delft, Netherlands — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [3]Materials Science, Rochester Institute of Technology, Rochester, NY, United States — [4]Air Force Research Lab, Wright-Patterson AFB, OH, United States

We present finite-temperature magnetic properties of FCC CoFeNiCr-based high entropy alloys (HEA). Particular emphasis is put on CoCrFeNiPd HEAs, which have T_Cs in the neighborhood of ambient [1]. T_Cs are computed employing density functional theory and a magnetic mean-field model [2]. Our theoretical results are in excellent agreement with experimental data revealing high predictive power of the employed theoretical method. The computational framework is used to explore the dominant mechanisms that determine T_C. Finally we propose alternative alloying strategies for tuning T_C towards room temperature. Our predicted "treasure maps" [2] narrow down the enormous configuration space for distinct magnetic properties of these multi-component alloys to a well-defined set of alloy compositions revealing a wide range of ferromagnetic properties and T_Cs near room temperature in hitherto unexplored alloys. [1] Belyea *et al.*, Sci. Rep. **5**, 15755 (2015); Lucas *et al.*, J. Appl. Phys. **109**, 07E307 (2011). [2] Körmann *et al.*, Appl. Phys. Lett. 107, 142404 (2015).

MM 11.6 Mon 17:30 H39

Ab initio prediction of sound velocities in planetary inner cores — •Jan W. Jaeken[1], Attilio Rivoldini[2], Tim van Hoolst[2], Veronique Van Speybroeck[1], Michel Waroquier[1], and Stefaan Cottenier[1,3] — [1]Center for Molecular Modeling, Ghent University — [2]Reference Systems and Planetology, Royal Observatory of Belgium — [3]Department of Materials Science and Engineering, Ghent University

Earth's inner core's sound velocities and acoustic anisotropy are well known through seismological observation. However, explaining this anisotropy has proven to be difficult. High pressure experiments are not easy to perform, especially when considering exoplanets with even

higher core pressures.

Ab initio modeling provides a tool for determining material properties when experiments are difficult or dangerous. We have studied the effect of stacking faults on the sound velocities of close-packed iron at high pressures. We show how the stacking sequence has a crucial effect on acoustic anisotropy.

The method outlined in this work is material-independent, making it a potentially valuable tool in the design of new materials with user-defined sound propagation properties.

MM 11.7 Mon 17:45 H39

Ab initio study on GaP-Si interface formation and properties — •Andreas Stegmüller and Ralf Tonner — Fachbreiech Chemie, Philipps-Universität, 35032 Marburg

In thin-film heterostructures, interfaces determine charge carrier transport and exciton trapping. Here, the GaP-Si interface was chosen as a model system to study the interface formation and associated properties eminent for constructing optoelectronic applications. Experimental findings are reported showing GaP-Si is neither flat nor abrupt but intermixed within 8 atomic layers and faceted.[1]

Abrupt and intermixed interfaces at (001), (111), (112) and (113) are discussed and absolute formation energies from DFT applying large slab- and bulk-type supercells are presented. We separately analyzed local and cell-wide (3-5 nm) features on the atomic structure (local stress vs. material strain), atomic charges (interface charge vs. bulk-like atomic polarization (NPA)), electrostatic potential (transition and convergence through an interface vs. III/V film polarization/oscillating field) and relate them to stability. However, as the materials should be considered covalent (not ionic) and dominated by local contributions, more chemically motivated arguments (e.g. electronegativity) are needed in order to see why simple, charge-based models [2,3] are only qualitatively correct.

[1] Andreas Beyer et al., submitted 2015.
[2] Walter A. Harrison et al., Phys. Rev. B, 18, 4402-4410, 1978.
[3] M. D. Pashley, Phys. Rev. B, 40, 10481-10487, 1989.