MA 13: Focus Session: Magnetism in Materials Science: Thermodynamics, Kinetics and Defects II (joint session MM/MA)

Sessions: Magnetism III and Magnetism IV

Time: Monday 15:45–18:45 Location: TC 010

Topical Talk MA 13.1 Mon 15:45 TC 010

Ferromagnetic Nuclear Resonance for studying defects in multilayers and nanocomposites : Structure and magnetic properties — •Christian Mény — IPCMS, 23 rue du loess 67034, Strasbourg, France

Nuclear Magnetic Resonance in Ferromagnets (also called Ferromagnetic Nuclear Resonance, FNR) is a rather unknown technique. However it can give very unique information in the study of defects in ferromagnetic films, multilayers, and nanocomposites. The yield of FNR experiments is twofold. On one hand the FNR spectrum reflects the distribution of hyperfine fields in the sample and thus gives information about the different chemical configurations and site symmetries in the sample,their structure and their defects (stacking faults, impurities, grain boundaries...). On the other hand the evolution of the spectral shape against the FNR radio frequency field strength probes the magnetic stiffness of the electronic moments around the nucleus site thus providing information comparable to that given by ferromagnetic resonance measurements. Therefore, combining both yields makes it possible to correlate the inhomogeneous magnetic properties of a sample to its different structural components and defects. A general presentation of FNR will be given in the first part of the presentation; the second part will be focused on the study of defects in nanostructures.

Reference: Y.F. Liu, , C. Meny; Sampling the structure and chemical order in assemblies of ferromagnetic nanoparticles by Nuclear Magnetic Resonance. Nat. Commun.7, 11532 (2016); and references therein.

MA 13.2 Mon 16:15 TC 010

First-principles study of interface energies in Fe-Al superalloy nanocomposites — •Ivana Miháliková[1,2], Anton Slávik[1,2], Martin Friák[1,2], David Holec[3], Nikola Koutná[1,2,4], Monika Všianská[1,5,6], and Mojmír Šob[5,1,6] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, Austria — [4]Institute of Materials Science and Technology, TU Wien, Vienna, Austria — [5]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [6]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Fe-Al nanocomposites with a superalloy-type of microstructure possess a great potential as an alternative to the currently used steel grades in high temperature applications. We employ *ab initio* calculations to analyze relations between ordering tendencies of Al atoms in the disordered Fe-18.75at.%Al phase on one hand and thermodynamic, structural and magnetic properties of Fe-Al-based nanocomposites on the other. The Fe-18.75at.%A supercells without 1st and 2nd nearest neighbor Al-Al pairs have a lower energy than those mimicking an ideal disorder (a special quasi-random structure, SQS). The same thermodynamic preference is found also in the case of coherent interfaces with {001}, {011} and {111} crystallographic orientations between Fe_3Al compound and Fe-Al phases with different atomic distributions.

MA 13.3 Mon 16:30 TC 010

Ab initio **study of magnetic states in superalloy nanocomposite phase Fe_2AlTi** — •Anton Slávik[1,2], Ivana Miháliková[1,2], Martin Friák[1,2], David Holec[3], Monika Všianská[1,4,5], and Mojmír Šob[4,1,5] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversitaet Leoben, Leoben, Austria — [4]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [5]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

The Fe_2AlTi intermetallic compound is one of Heusler $L2_1$-structure materials possessing interesting magnetic properties. We study thermodynamic, electronic, structural and elastic properties of different magnetic states in Fe_2AlTi by *ab initio* fixed-spin-moment calculations. A spin-polarized ferrimagnetic state with the magnetic moment of 0.925 μ_B per formula unit is found to be a stable energy minimum at T=0 K. Interestingly, a non-magnetic state has its total energy only by 10.6 meV/atom higher and, consequently, the lowest energy state is found very sensitive to different perturbations. We discuss this weak stability in the case of fairly high statistical probability of occurrence of the non-magnetic state, trigonal strains (to which Fe_2AlTi has a compression-tension asymmetric response), off-stoichiometry and point defects as well as interfaces within Fe-Al-Ti superalloy nanocomposites.

MA 13.4 Mon 16:45 TC 010

Energetics of non-stoichiometric stacking faults in Fe-Nb alloys: An ab initio study — •Ali Zendegani[1], Michaela Šlapáková Poková[2], Christian Liebscher[2], Frank Stein[2], Alvin Noe Collado Ladines[3], Thomas Hammerschmidt[3], Ralf Drautz[3], Fritz Körmann[1], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Charles University, Prague, Czech Republic — [3]ICAMS, Ruhr-Universität Bochum, Bochum, Germany

The microstructure in structural materials plays an essential role for their mechanical properties. In Fe-Nb alloys a hardening via TCP phases (e.g. Laves Fe2Nb and Fe7Nb6) can be achieved. At the same time, various types of stacking faults occur during deformation. In the present work, we investigate the correlation of both features in the C14 Fe2Nb Laves phase. For this purpose, density functional theory calculations are combined with thermodynamics concepts. Particular care has been taken to take atomic relaxation effects and magnetic degrees of freedom into account. We proof that excess Nb will segregate to these planar defects and result in a local phase transformation next to it. The energetics of these structures are compared to the phase separation as predicted by the bulk phase diagram. Comparing our results with high-quality TEM measurements has revealed that some of the complex crystal structures next to basal and pyramidal stacking faults are in a constrained state.

30 min. break

Topical Talk MA 13.5 Mon 17:30 TC 010

Improving the finite-temperature description of magnetic materials — •Anders Bergman — Department of Physics and Astronomy, Uppsala University,Uppsala, Sweden

State-of-the-art simulations based on electronic structure theory and atomistic models have now evolved to a point where computer-guided materials design has become a realistic option for many classes of materials. In this talk we will introduce improvements to the standard description of finite-temperature magnetism with the aim of increasing the predictive capability of these simulations further.

We present an extended atomistic spin model obtained by augmenting the Heisenberg Hamiltonian to take longitudinal fluctuations of the magnetic moments into account. This is done by parametrisation from a first-principles basis, interpolating from low-temperature ferromagnetic and high-temperature paramagnetic reference states. The method gives a good agreement of Curie temperatures and paramagnetic properties compared with experiments as well as similar, earlier theoretical models.

Introducing quantum statistics into atomistic simulations has been shown to improve the observed temperature dependence of the magnetisation and of the magnetic specific heat. This allows for a more realistic modelling of the magnetic contribution to the free energy and thus a better description of phase-stabilities and related properties. We present how the quantum statistics can be modelled with varying levels on complexity and demonstrate the method for both elemental systems and magnetic alloys.

MA 13.6 Mon 18:00 TC 010

Interplay between magnetic and energetic properties in FeMn alloys from first principles — •Anton Schneider[1], Chu Chun Fu[1], Cyrille Barreteau[2], and Frédéric Soisson[1] — [1]CEA,

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Iron-based alloys play a central role in several technological applications. In these alloys, the magnetism has an important impact on thermodynamic and kinetic behaviors, and on the properties of point defects. Especially, iron-based alloys may exhibit complex magnetic structures if the magnetic ordering tendency of the alloying element in its pure phase differs from that of iron.

Iron-Manganese bcc alloys are studied using Density Functional Theory (DFT) in order to elucidate the correlation between the magnetic structures, and the energetics of Mn atoms and clusters in the presence of vacancies and interstitial impurities. The FeMn alloys exhibit well distinct magnetic interactions between the Fe atoms and the Mn solutes depending on local chemical environments, which are rationalized in terms of electronic structures. Both low-energy magnetic collinear and non-collinear states are investigated.

The DFT results are then used to parameterize new Heisenberg-like models, in the presence of vacancies, aiming at investigating the finite-temperature magnetic effects employing Monte Carlo simulations. A particular attention is given to the role of magnetic short-range order on the vacancy formation energy, as a function of temperature.

MA 13.7 Mon 18:15 TC 010

Machine Learning assisted Heisenberg model for systems with ill-defined pairwise magnetic interactions — •Osamu Waseda, Omkar Hegde, and Tilmann Hickel — MPIE

Magnetic interactions are important for the stability of structural phases as well as for various thermophysical effects such as magnetocalorics. In order to determine their free energy contribution in Fe-based materials, the Heisenberg model has been used as a handy method for decades. Despite its simplicity, there is little experience with the application of this model to systems containing various types of atoms and/or structural defects, as their interaction parameters cannot be defined straightforwardly. In this study, data sets for Fe-Mn systems containing structural defects are created from spin-polarized DFT calculations. They are then translated into the Heisenberg parameters via Ridge regression. Finally, the contribution of the magnetic interactions to the specific heat is determined through Monte Carlo simulations.

MA 13.8 Mon 18:30 TC 010

Numerical simulation of spin fluctuations in materials science: magnetic bond-order potentials and hybrid Monte Carlo — •Ning Wang, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

The finite-temperature properties of many magnetic materials are to a large degree influenced by spin fluctuations. The numerical simulation of these effects, however, faces several obstacles. In particular, the modelling of the magnetic interactions at the quantum-mechanical level should be neither oversimplified nor too computationally expensive. Furthermore, an efficient numerical sampler is required in order to treat the high-dimensional integration problem of the thermal expectation values. Our modelling approach are analytic bond-order potentials based on tight-binding. To treat the sampling problem, we extended the hybrid Monte Carlo sampler so that it will also work for the classical spin system. We furthermore developed an auxiliary-Hamiltonian method in order to improve the sampling efficiency. With this methodology, we simulate the magnetic phase transitions in BCC iron and determine the magnetic free energy difference between the BCC and FCC states of iron.