MM 5: Topical session (Symposium EPS and MM, joint session with MA): Magnetism in Materials Science: Thermodynamics, Kinetics and Defects (joint session MM/MA)

Sessions: Magnetism I and Magnetism II

EPS-Symposium organized by Chuchun Fu (CEA-Saclay, Gif-sur-Yvette, France), Thomas Hammerschmidt (Ruhr-Universität Bochum, Germany), Tilmann Hickel (MPI Eisenforschung, Düsseldorf, Germany), and Véronique Pierron-Bohnes (IPCMS CNRS-Unistra, Strasbourg, France).

Time: Monday 10:15–13:15 Location: TC 010

Topical Talk MM 5.1 Mon 10:15 TC 010

First principles many-body calculations for rare earth-based materials: present status and open challenges — •Silke Biermann — Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau, France

Rare earth compounds are at the heart of a wide range of modern materials applications, ranging from permanent magnets to pigments, and reliable and efficient first principles descriptions of their properties are highly desirable in view of the development of rational design techniques. Strong local Coulomb interactions on the rare earth f-shell, however, make ab initio calculations for such materials challenging.

We will review the present status of dynamical mean field theory-based approaches to the problem and describe recent methodological developments in the field [1,2,3].

[1] P. Seth, P. Hansmann, A. van Roekeghem, L. Vaugier, S. Biermann, Physical Review Letters 119 056401 (2017). [2] Pascal Delange, Silke Biermann, Takashi Miyake, Leonid Pourovskii, Phys. Rev. B 96, 155132 (2017). [3] S. Panda, L. Pourovskii, S. Biermann, in preparation.

MM 5.2 Mon 10:45 TC 010

Continuous transition from antiferro- to ferromagnetic state via moment canting in $Ni_{2-x}Co_xMnAl$ — •Michael Leitner[1], Pascal Neibecker[1], Matthias Opel[2], Xiao Xu[3], Ryosuke Kainuma[3], and Winfried Petry[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [3]Department of Materials Science, Tohoku University, Sendai 980-8579, Japan

The magnetic structure of materials is often discussed only in terms of the classical concepts of ferromagnetism and antiferromagnetism, however, interesting phenomena can be expected when a system is driven to the boundary between these regimes by adjusting external parameters. B2-ordered $Ni_{2-x}Co_xMnAl$ is a case in point: Ni_2MnAl, a potential ferromagnetic shape-memory material, displays antiferromagnetism [1], while NiCoMnAl, predicted to be a halfmetal, is ferromagnetic [2].

We have studied this system for $0 \leq x \leq 0.8$. Temperature-dependent neutron powder diffraction proves an antiferromagnetic ordering for $x < 0.4$, while the macroscopic magnetization shows an increasing longitudinal component for all $x > 0$. We argue that this constitutes a continuous, spatially homogeneous transition from antiferro- to ferromagnetism via canted spins, which is reproduced by a simple Heisenberg model.

[1] M. Acet et al., *J. Appl. Phys.* **92**, 3867 (2002)
[2] P. Neibecker et al., *Phys. Rev. B* **96**, 165131 (2017)

MM 5.3 Mon 11:00 TC 010

Modeling the high-temperature paramagnetic state of magnetic materials from first-principles - coupling of lattice vibrations and disordered magnetism — •Björn Alling[1,2] and Irina Stockem[1,2] — [1]Linköping University, Sweden — [2]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The paramagnetic state of magnetic materials lack global magnetization and long range order between moments. However, in most cases there still exist important local magnetic moments. Also, lattice vibrations are important for properties and stability of materials at high temperature. Simultaneous presence of disorder of magnetic and vibrational nature poses a severe challenge for first-principles theory.

I present our recently developed method combining atomistic spin dynamics with ab-initio molecular dynamics (ASD-AIMD) treating the magnetic and vibrational degrees of freedom on an equal, first-principles based footing. It allows us to explicitly study the coupled dynamics of magnetism and lattice in the paramagnetic state.

We use it to study paramagnetic CrN. Phonon life times are obtained from the AIMD part of the simulations. At 300 K, we see dramatically lower phonon lifetimes as compared to an adiabatic, fast-magnetism, approximation. Further, the phonon lifetime does not decrease in the normal manner with increasing temperature which could explain anomalys thermal conductivity observed experimentally for many materials in the paramagnetic state. These results underline the importance of allowing for a dynamical coupling between magnetism and lattice vibrations in theoretical studies of the paramagnetic state.

MM 5.4 Mon 11:15 TC 010

Lattice relaxations in paramagnetic materials from first principles — •Davide Gambino[1] and Björn Alling[1,2] — [1]Department of Physics, Chemistry, and Biology (IFM) Linköping University, SE-58183 Linköping, Sweden — [2]Max-Planck-Institut für Eisenforschung GmbH, D-402 37 Düsseldorf, Germany

The first-principles calculation of many material properties starts with the relaxation of the atomic positions of the system under investigation. This procedure is routine for nonmagnetic materials, as well as for magnetically ordered compounds. However, when it comes to magnetically disordered systems, it is not clear what geometry one should take into account. Here we propose a method for the structural relaxation of magnetic materials in the paramagnetic regime within the disordered local moment (DLM) picture in the framework of density functional theory (DFT). The method can be easily implemented using any ab initio code.

We consider as a test case Fe vacancy in bcc Fe in the paramagnetic regime: as a result, the nearest neighbors to the vacancy relax inwards of about 0.16 Angstrom (-5% of the ideal bcc nearest neighbor distance), which is twice as large as the relaxation in the ferromagnetic case, and the vacancy formation energy calculated on these positions results to be 1.60 eV, which corresponds to a reduction of about 0.1 eV compared to the formation energy calculated on ferromagnetic-relaxed positions. Our results are in good agreement with recent DFT+DMFT calculations and with experimental values. Other systems under investigations are interstitial defects in bcc Fe and FeCr random alloys.

15 min. break

Topical Talk MM 5.5 Mon 11:45 TC 010

We need perfect defects - challenging the Brown's paradox in permanent magnetism — •Oliver Gutfleisch — TU Darmstadt, Materialwissenschaft

It is common understanding that among the intermetallic phases used for high performance permanent magnets, practically none can fully realize its potential based on the intrinsic magnetic properties. Even if the grain size of the fully-dense magnet is close to the single domain size, the coercivity Hc is usually one order of magnitude smaller than the anisotropy field Ha - this situation is known as Brown's paradox. The presence of crystallographic defects of various kinds, of secondary phases, of surface imperfections as well as magnetic inhomogeneities leads to local magnetic softening. On the other hand, a perfect single crystal shows 'no' coercivity whatsoever. Looking at nucleation-type NdFeB (1,2) and pinning type SmCo (3) magnets we will revisit the Brown's paradox and discuss possible ways of overcoming it.

1 Helbig et al., Experimental and Computational Analysis of Magnetization Reversal in (Nd,Dy)-Fe-B Core Shell Sintered Magnets, Acta Materialia 127 (2017) 498.
2 Loewe et al., Grain boundary diffusion of different rare earth elements in Nd-Fe-B sintered magnets by experiment and FEM simulation, Acta Materialia 124 (2017) 421.
3 Duerrschnabel et al., Atomic structure and domain wall pinning in samarium -cobalt based permanent magnets, Nature Communications 8:54 (2017).

Topical Talk MM 5.6 Mon 12:15 TC 010

Interplay of moment-volume and electron-phonon coupling in the itinerant electron metamagnet $LaFe_{13-x}Si_xH_y$ — •Markus Ernst Gruner — Faculty of Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen, Germany

$LaFe_{13-x}Si_xH_y$ compounds belong to the most promising systems for room temperature magnetic refrigeration. Here, large adiabatic temperature and isothermal entropy changes in an external magnetic field are obtained at a first-order metamagnetic transition. It is accompanied by a large volume change without change in lattice symmetry, attributed to the competition of different magnetic states of Fe associated with varying atomic volumes. Recently, we detected by first-principles lattice dynamics and nuclear resonant inelastic X-ray scattering characteristic changes in the vibrational density of states at the magnetic transition in $LaFe_{13-x}Si_x$, which involves the disappearance of a high-energy peak in connection with an overall softening of phonons in the paramagnetic phase. This contributes to the good magneto- and barocaloric properties of the material, in terms of a cooperative contribution of magnetic, electronic and vibrational degrees of freedom to the entropy change. The softening originates from adiabatic electron-phonon coupling caused by specific changes in the electronic density of states at the Fermi level, which are sensitive to the magnitude of the Fe moment, rather than to magnetic order. Finally, we demonstrate that the same mechanisms are effective in the hydrogenated compound at ambient conditions.
Funding by the DFG within SPP 1599 is gratefully acknowledged.

MM 5.7 Mon 12:45 TC 010

Spin-lattice effects in $LaFe_{11.6}Si_{1.4}$ revealed by powder diffraction — •Tom Faske[1], Wolfgang Donner[1], and Markus Hölzel[2] — [1]TU Darmstadt, Materials Science, Structure Research, Darmstadt, Germany — [2]Heinz Maier-Leibnitz Zentrum, Garching, Germany

$LaFe_{13-x}Si_x$ ($x = 1.0 - 1.6$) is a promising material class for application in magnetic cooling and has been extensively studied in recent years. For $x \leq 1.6$ it exhibits a first order magneto-structural phase transition around 200 K which becomes second order for $x > 1.6$. The first-order transition is accompanied by a large isothermal entropy change $|\Delta S_{iso}|$ in conjunction with a high adiabatic temperature change $|\Delta T_{ad}|$, which are both important figures of merit for a potential magnetocaloric application.

Here we report on the detailed study of the first-order phase transition of $LaFe_{13-x}Si_x$ by means of temperature and magnetic field dependent x-ray and neutron powder diffraction. External magnetic fields increase the Curie temperature by ≈ 4 K/T, so that the phase transition could be induced thermally and by applying magnetic fields of up to 5 T during the diffraction experiments. In a narrow magnetic field and temperature range, both phases were present in the diffraction patterns. Subtle structural differences in the two-phase region between the magnetic field and temperature induced phase transitions revealed a change in the entropy transfer of the two systems.

MM 5.8 Mon 13:00 TC 010

Symmetry breaking induce robust monoclinic-distortion and unconventional charge ordering at room temperature in single crystal of Na2.7Ru4O9 — •Arvind Yogi[1,2], C. I. Sathish[1,2], Hasung Sim[1,2], Y. Noda[3], and Je-Geun Park[1,2] — [1]Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul 08826, Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [3]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan

We discovered by combining the results of SC-XRD, electrical resistivity, specific heat, and susceptibility that Na2.7Ru4O9 with the monoclinic new tunnel type lattice (space group P 21/m) evolves an unprecedentedly charge ordering (CO) at room temperature while retaining of metallicity. The temperature dependent SC-XRD results shows super-lattice peaks q1 (0, 1/2, 0) and q2 (0, 1/3, 1/3), that causes the translation symmetry breaking of the lattice which induces robust monoclinic-distortion at room temperature, is the evidence for the formation of an unconventional charge ordering (CO). Na2.7Ru4O9 show a first-order phase transition in the electrical resistivity with two consecutive transitions at Tc (1) = 365 K and Tc (2) = 345 K for Na2.7Ru4O9 which supports well by magnetization and heat-capacity results. The electron-phonon mediated scattering mechanism is involved in the resistivity. We argue that the origin of unprecedented CO is due to the localized 4d electrons.