# MA 30: Magnetic Materials II

Time: Wednesday 15:00–17:00 Location: H 0112

MA 30.1 Wed 15:00 H 0112

**Pure spin thermocurrents in Permalloy at high Temperatures** — •Marco Di Gennaro[1], Bin Xu[2], and Matthieu Verstraete[1] — [1]Department of Physics, University of Liege, B4000 Liege — [2]Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, Arkansas 72701, USA

We present a method for the calculation of spin dependent transport quantities in ferromagnetic metals based on an variational resolution of the semi-classical Boltzmann equation. The electron-phonon coupling is calculated ab-initio [1], explicitly considering two different spin channels and thermal expansion. The calculated Seebeck coefficient for magnetic Permalloy agrees with experimental data measured within a large temperature range. We also calculate the spin dependent Seebeck coefficient describing a build up of spin chemical potential under application of a temperature gradient. We find that a thermal gradient can produce a pure spin current in Permalloy at high temperatures.

[1] B. Xu and M. J. Verstraete, Phys. Rev. Lett. 112, 196603 (2014).

MA 30.2 Wed 15:15 H 0112

**Finite-temperature magnetism and transport properties of FeRh** — •Sergiy Mankovsky[1], Svitlana Polesya[1], Kristina Chadova[1], Diemo Ködderitzsch[1], Jan Minar[1], Julie B. Staunton[2], and Hubert Ebert[1] — [1]Dept. Chemie/Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Deutschland — [2]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

The finite temperature magnetic properties of the FeRh compound with B2 structure have been investigated by performing first-principles electronic structure calculations in combination with Monte Carlo simulations. The central role of the temperature dependence of the interatomic exchange interactions for the AFM-FM phase transition at $\approx 340K$ is demonstrated, where the $J_{ij}(T)$ dependence is determined by the degree of magnetic order in the system. The finite temperature electric conductivity has been calculated using the scheme based on the alloy analogy model. Investigation of separate contributions to the electric conductivity shows explicitly the strongly dominating role of thermal spin fluctuations. The influence of impurities and intermixing between Fe and Rh sub-lattices on the magnetic and transport properties is investigated. The results are compared with the experimental data showing rather good agreement.

MA 30.3 Wed 15:30 H 0112

**Effect of annealing on the magnetic state in Ni-doped FeRh alloys** — •Alisa Chirkova[1,2,3], Alexander Funk[1], Anja Waske[1], Konstantin Nenkov[1], Ludwig Schultz[1], Nikolai Baranov[2,3], and Thomas George Woodcock[1] — [1]IFW Dresden, Dresden, Germany — [2]Institute of Metal Physics, Yekaterinburg — [3]Ural Federal University, Yekaterinburg

FeRh alloys are known for the antiferromagnetic (AF) - ferromagnetic (FM) phase transition which takes place at about 360 K on heating; the crystal symmetry of CsCl-type ($\alpha'$) is retained. The transition temperature $T_t$ can be changed by additions of other d-metals [1]; Ni shifts $T_t$ down to about 150 K and at 2 at. % Ni only the FM state exists. Hydrostatic pressure raises $T_t$ and in Ni-doped samples the effect is stronger. Depending on the cooling rate after long term annealing, either AF or FM states were produced in $(Fe_{0.965}Ni_{0.035})_{49}Rh_{51}$ samples at 2 K. Quenching produced the AF state, whereas cooling at 1 K/min resulted in the FM state. Microstructural analysis revealed the presence of retained high temperature $\gamma$ phase. The $\gamma$ phase is paramagnetic, Rh-rich (60 at.%) and contains twice as much Ni as $\alpha'$. The quenched (AF) sample has 0.070 volume fraction of the $\gamma$ phase against 0.035 in the slow-cooled (FM) sample which indicates that Ni content of the $\alpha'$ phase differs between the samples, thus explaining the different magnetic state. The possible additional effect of strain on the phase boundaries will also be considered.

[1] N.V. Baranov, E.A. Barabanova, J. Alloys Compd. 219 (1995) 139.

MA 30.4 Wed 15:45 H 0112

**Structural and magnetic properties of $Fe_{11-x}Co_xTiCe$ intermetallic compounds** — •Dagmar Goll, Ralf Loeffler, Roland Stein, Ulrich Pflanz, Susanne Goeb, Roman Karimi, and Gerhard Schneider — Aalen University, Materials Research Institute (IMFAA), Aalen

Ce-based hard magnetic intermetallic compounds are currently undergoing a revival for potential low-cost permanent magnet applications due to the better abundance of Ce in the earth crust compared to Nd or Dy. One of these compounds is $Fe_{11}MCe$ (M: Ti, Mo, V, Cr) with tetragonal $Mn_{12}Th$ (12:1) structure and uniaxial anisotropy. The novel quaternary compound $Fe_{11-x}Co_xTiCe$ with Co content $x = 0$ to 3.25 (0 at% to 25 at%) has been fabricated by arc melting. The samples have been analyzed concerning their crystallographic structure and intrinsic magnetic properties as function of temperature using x-ray diffraction, domain pattern analysis and magnetometry. With increasing Co content the lattice structure becomes contracted and the Curie temperature $T_C$ continuously increases from 468 K (0 at% Co) to 725 K (25 at% Co). The maximum values of the anisotropy constant $K_1$ and saturation polarization $J_s$ are observed for a Co content of 15 at%. For about $x = 1.95$ (about 15 at% Co) $K_1$ and $J_s$ are 2.15 MJ/m$^3$ and 1.27 T at room temperature and 1.22 MJ/m$^3$ and 1.05 T at 200 °C, respectively.

MA 30.5 Wed 16:00 H 0112

**Electron-electron interaction strength in ferromagnetic nickel determined by spin-polarized positron annihilation** — •Hubert Ceeh[1], Josef-Andreas Weber[1], Michael Leitner[1], Liviu Chioncel[2], Dieter Vollhardt[2], Diana Benea[3], Peter Böni[1], Hubert Ebert[3], Jan Jan Minár[3], and Christoph Hugenschmidt[1] — [1]Technische Universität München, Physik Department, Lehrstuhl E21, James-Franck-Straße, D-85748 Garching, Germany — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [3]Chemistry Department, University Munich, Butenandstraße 5-13, D-81377 München, Germany

Spin resolved positron annihilation measurements using the angular correlation of annihilation radiation technique have been performed on ferromagnetic Ni. The analysis is based on a direct comparison of the experimentally obtained projections of the momentum density and state-of-the-art dynamic mean-field calculations. The experimental data were best described for a value of 2.0 eV for the on-site repulsion term $U$ in the Hubbard model. We show that spin-polarized 2D-ACAR, where probe effects of the positron can be avoided, is a powerful tool to investigate the electronic structure of ferromagnetic systems.

MA 30.6 Wed 16:15 H 0112

**Large magnetic anisotropy in $LaCo_{5-x}$** — •Christoph Schwöbel[1], Konstantin Skokov[1], Michael Kuzmin[2], and Oliver Gutfleisch[1,3] — [1]TU Darmstadt, Germany — [2]IM2NP, Marseille, France — [3]Fraunhofer IWKS, Hanau, Germany

One focus in the search for new hard magnetic materials are compounds which exhibit a large magneto-crystalline anisotropy as the anisotropy field represents the upper limit for the potential coercive field in a permanent magnet. Materials which crystallize in a hexagonal structure like the $CaZn_5$-structure can exhibit an easy axis along the c-direction with a relatively high anisotropy field. The investigated $LaCo_5$ system is particularly interesting as the magnetic moment comes solely from the Co atoms. Therefore it is possible to gain further insight on the magnetism of this 3d element.

Single crystals with a substoichiometric composition of $LaCo_{5-x}$ were grown and investigated. The measurements were performed up to 14 T at different temperatures. Anisotropy fields larger than 20 T were extrapolated.

MA 30.7 Wed 16:30 H 0112

**Giant magnetic anisotropy and quantum tunneling of the magnetization in $Li_2(Li_{1-x}Fe_x)N$** — •Anton Jesche[1] and Paul C. Canfield[2] — [1]Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86135 Augsburg, Germany — [2]Ames Laboratory, Iowa State University, Ames, Iowa 50011, USA

The magnetic anisotropy of 3d transition metals is usually considered to be weak. Main reason is the widely known paradigm of orbital quenching. However, a rare interplay of crystal electric field effects and spin-orbit coupling causes a large orbital contribution to the magnetic moment of iron in $Li_2(Li_{1-x}Fe_x)N$. This leads not only to large magnetic moments of $\sim 5\,\mu_B$ per iron atom but also to an enormous magnetic anisotropy field that extrapolates to more than 200 Tesla [1]. Magnetic hysteresis emerges for $T < 50\,K$ and the coercivity fields of more than 11 Tesla exceed even the hardest 4f electron based ferromagnets.

$Li_2(Li_{1-x}Fe_x)N$ not only has a clear and remarkable anisotropy, generally not associated with iron moments, but also shows time-dependence more consistent with molecular magnets. In particular for low iron concentrations $x \ll 1$ the spin-inversion is dominated by a macroscopic tunneling process rather than by thermal excitations.

It is shown that the huge magnetic anisotropy makes $Li_2(Li_{1-x}Fe_x)N$ (i) an ideal model system to study macroscopic quantum effects at elevated temperatures and (ii) a basis for novel magnetic functional materials.

[1] A. Jesche *et al.* Nature Commun. 5:3333 (2014)

MA 30.8 Wed 16:45 H 0112

**Magnetic anisotropy manipulation in Ni nanostructures fabricated on $VO_2$ (100) thin films imaged by time-resolved high resolution x-ray microscopy across the phase transition** — •Simone Finizio[1], Mehran V. Khanjani[1], Andrea Fantini[1,2], Michael Foerster[3], Simone Altendorf[2,4], Donata Passarello[2], Lucia Aballe[3], Stuart S.P. Parkin[2], and Mathias Kläui[1] — [1]Institut für Physik, Universität Mainz, Mainz, Germany — [2]IBM Almaden Research Center, San Jose, CA, USA — [3]ALBA Synchrotron Light Source, Cerdanyola del Valles, Spain — [4]Max Planck Institute for Microstructure Physics, Halle, Germany

Due to the possibility to generate strain variations on ultra-short timescales, the metal-insulator-transition (MIT) in $VO_2$ is of particular interest for the study of the dynamics involved in the magnetostrictive coupling. In particular, strain can be manipulated in conventional piezoelectric materials only on slow timescales (<GHz), while here fast strain variations result from the MIT, which occurs on the ps timescale.

In this contribution, we will present x-ray magnetic microscopy imaging of Ni nanostructures fabricated on $VO_2$ (100) thin films deposited by pulsed-laser-deposition on $TiO_2$ (100) substrates upon crossing the MIT of the $VO_2$. Due to strain change when crossing the MIT, strong changes in the magnetic anisotropy of the Ni nanostructures were observed, which changed from a low temperature uniaxial-anisotropy dominated state to a high temperature shape-anisotropy dominated state.