MM 16: Transport - Heat Transport and Thermoelectricity

Time: Monday 17:00–18:00 Location: IFW A

MM 16.1 Mon 17:00 IFW A

Specific heat capacity measurements and transmission electron microscopy investigation of FeMn alloys — •Marius Gerlitz, Martin Peterlechner, Sergiy Divinski, and Gerhard Wilde — Westfälische Wilhelms-Universität, Münster, Deutschland

Magnetocaloric materials are promising for various fields of application and their thermodynamic fundamentals are crucial to understand. In this work, low temperature specific heat capacity measurements are performed for a series of Fe-Mn alloys with and without application of a magnetic field (up to 9T) in the temperature interval from 4 K to 400 K. A physical properties measurement system (PPMS) is used and the 2-tau method is applied for the analysis. Furthermore, the heat capacity measurements are extended to higher temperatures from 300 K to 723 K using differential scanning calorimetry and applying heating rates of 20 K/min. As a result, thermal and magnetic entropy contributions are determined alongside with the determination of further characteristic properties such as the Debye temperature or the electronic contribution to the specific heat. A microstructural analysis is performed by transmission electron microscopy (TEM). The results are discussed with respect to the chemical composition and potential short-range ordering.

MM 16.2 Mon 17:15 IFW A

Thermal conductivity of Th and ThC — •Lukas Kyvala and Dominik Legut — VSB - Technical University of Ostrava, 17. listopadu 15, 70833 Ostrava-Poruba, Czech Republic

Thermal conductivity is one of the most important properties of nuclear fuel materials affecting many processes such as swelling, grain growth, and fission gas release and limits the transfer of the linear power.

Experimental measurement of thermal conductivity is difficult because of the loss of heat through convection, conduction, and radiation. The different measurements do not find full agreement even for such a simple case like silicon. Moreover, the measurement of radioactive elements is complicated due to the self-heating. Theoretical calculations are then a very useful tool.

We demonstrate the success of predicting the thermal conductivity of potential nuclear fuels like Th and ThC using electron-structure calculations. Both phonon (lattice) and electron contributions were calculated as a function of temperature.

Next, we discuss why the total thermal conductivity of thorium metal is more than twice as large as thorium monocarbide and why the optical phonon modes of ThC accounting only for approximately 6 % of the total phonon contribution. This result differs significantly from NpO_2 where the optical branches contribute only 27 %.

MM 16.3 Mon 17:30 IFW A

Temperature and doping dependence of the thermoelectric power of $Yb(Rh_{1-x}Co_x)_2Si_2$ intermetallic compounds — •Veljko Zlatic[1] and Ulrike Stockert[2] — [1]Department of Physics, Faculty of Science, University of Split, Croatia — [2]MPI for Chemical Physics of Solids, Dresden, Germany

The temperature and doping dependence of transport coefficients of $Yb(Rh_{1-x}Co_x)_2Si_2$ series of alloys is explained by an asymmetric Anderson model which takes into account the exchange scattering of conduction electrons on Ytterbium ions and the splitting of $4f$-states by the crystalline electric field (CEF). The substitution of rhodium by cobalt is described as an increase of chemical pressure which reduces the exchange coupling and the CEF splitting. The scaling analysis and numerical NCA solution of the model show that, at a given temperature, the effective degeneracy of the $4f$-state depends on the relative magnitude of the Kondo scale and the CEF splitting. The temperature and doping dependence of the thermopower of $Yb(Rh_{1-x}Co_x)_2Si_2$ series of alloys is explained as an interplay of quantum fluctuations, driven by the exchange scattering, and thermal fluctuations which populate the excited CEF states. The theoretical results obtained in such a way capture all the qualitative features of the experimental data.

MM 16.4 Mon 17:45 IFW A

Thermoelectricity in high-valley multiplicity materials — Roberta Farris[1], Francesco Ricci[2], Geoffroy Hautier[2], Gian-Marco RIgnanese[2], and •Vincenzo Fiorentini[1] — [1]Dip. di Fisica, Università di Cagliari, Italy — [2]University of Louvain-la-Neuve, Belgium

We present a detailed theoretical study of two promising thermoelectrics, LaSO and YB4Mo, which turn out to have a large multiplicity and band complexity factor from a data mining search on a large electronic-structure database. Bands are computed ab initio and transport is studied in the Bloch-Boltzmann approximation; lattice thermal is modeled from the ab initio harmonic spectrum. The two materials reach a ZT of over 2 at typical temperatures.