Contribution ID: **14** Type: **Contributed**

Inelastic neutron scattering on magnetocaloric compound $MnFe_4Si_3$

Thursday 21 July 2016 09:50 (20 minutes)

The magnetocaloric cooling process is based on the magnetocaloric effect (MCE) where entropy changes of a magnetic material in an applied magnetic field are tied to adiabatic changes in temperature. An entropy transfer between crystal lattice and the magnetic spin system has to take place. A large MCE at room temperature and low magnetic field for a material with abundant and environmentally friendly elements opens the way for magnetic cooling devices.
The ferromagnetic compound MnFe4Si3 belongs to the series Mn5-xFexSi3 and is a promising candidate material for such devices. It has a magnetic phase transition TC at about 300K and shows a moderate MCE of 2.9J/(kg K) at a reasonable magnetic field change from 0 to 2T [1,2,3].
Up to now experimental studies focussed mainly on the atomic and magnetic structure of this compound and revealed an unusual temperature dependence of the lattice parameters and possibly marked different magnitudes of ordered magnetic moments on different magnetic sites [1,3]. To add to the understanding of the fundamental driving forces of the MCE inelastic neutron and inelastic X-ray scattering experiments have been undertaken on the selected compound MnFe4Si3 to study the spin and lattice dynamics and their interactions. Magnon and acoustic phonon dispersion curves were obtained in the low energy regime (E<20meV) combining inelastic X-ray and inelastic polarized neutron measurements. Experiments reveal a strong anisotropy between in and out-of-plane magnetic interactions. Comparing the experimentally determined phonon dispersion with on-going DFT calculations will help us to understand the electronic ground state of the system. Presently, spin wave calculations are being performed in order to extract relevant exchange couplings.
Investigations of the paramagnetic scattering above TC in complement to the spin wave studies reveal sizable magnetic fluctuations in a large temperature range which are found to be isotropic. Characteristic length and energy scales will allow to address the question of the nature of its magnetism, e.g., itinerant versus localized.
The study of the inelastic properties under the influence of different external parameters like magnetic field or temperature might be an essential step towards the understanding of the mechanism of MCE in this substance.
[1] P. Hering et al., Chem. Mat. B 27, 7128 (2015), [2] A. Candini et al., J. Appl. Phys. 95, 6819 (2004), [3] O. Gourdon et al., J. Solid State Chem. 216, 56 (2014).

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Session Classification: Session IX: Thermoelectrics & Magnetocalorics (Chair: Karin Schmalzl)

Track Classification: Energy storage & transformation