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Pressure and temperature dependence of nuclear structure and magnetic properties in Mn4FeSi3

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Magnetic refrigeration based on the magnetocaloric effect holds a potential to replace conventional vapor compression cooling [1]. Compared to other magnetocaloric materials, the compounds in the system Mn5-xFexSi3 have the advantage that they do not contain expensive rare earth elements like Gd, nor toxic elements like As. After characterizing the compound MnFe4Si3 regarding structure and magnetism [2] another compound -namely Mn4FeSi3- of the system is now in the focus of our attention. Around the transition temperature of a magnetic phase transition it is supposed to undergo a structural phase transition from a hexagonal structure to an orthorhombic structure [3]. Investigation of both compounds and comparison of them might help understanding the underlying mechanism of the MCE in multiple site driven magnetocaloric materials, as the magnetic elements Manganese and Iron are distributed on at least two sites.

We performed neutron and x-ray powder diffraction experiments as a function of temperature on Mn4FeSi3 and could confirm that the magnetic transition at approx. 65 K is accompanied by a change in the symmetry presumably from P63/mcm to Cmcm indicating a close connection between lattice and spin degrees of freedom.

Synchrotron powder experiments varying pressure and temperature simultaneously were performed to follow the magnetic and associated structural transition. Volume changes and c/a ratio from both temperature and pressure dependant experiments clearly show that the influence of temperature is significantly stronger than the influence of hydrostatic pressure in this caloric material.
We were able to grow a large single crystal of the compound using the Czochralski Mehtod. Pressure dependent laboratory single crystal diffraction shows anomalies in the pressure dependence of the interatomic distances.
Macroscopic magnetization measurements performed on oriented single crystals of Mn4FeSi3 are currently being performed and will allow characterization of the anisotropy of the magnetic response of the material.

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[2] P. Hering, et al., Chem. Mater., 27 (20), 7128–7136 (2015).

[3] A. Candini, et al., J. of Appl. Phys. 95, 6819-6821 (2004).

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