

Structure property relationships in magnetocaloric materials

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Magnetic cooling based on the magnetocaloric effect could replace conventional vapor compression cooling, as it has potentially lower energy consumption and is free from gases hazardous to the environment like fluorinated hydrocarbons.

Suitable materials used for this technology exhibit a sizeable magnetocaloric effect (MCE), i.e. they show a considerable temperature change when exposed to a magnetic field. The MCE is particularly large when a transition to a magnetically ordered phase is accompanied by a structural transition, which, however, can reduce the cyclability of the material. The search for suitable materials is still ongoing as there are other demanding requirements (e.g. good moulding behaviour, cheap and non-toxic constituent elements, small hysteresis at the magnetic transition for the materials, tunable transition temperature). From the fundamental point of view there are still many open questions regarding the underlying mechanism of the magnetocaloric effect, in particular with respect to the coupling of the spin and lattice system.

One of the structural characteristics of magnetocaloric materials is the existence of two (or more) crystallographically independent sites for the paramagnetic atoms within the crystal structure. In addition, most of the magnetocaloric materials show a pronounced magnetic anisotropy and a clear response of the crystal lattice at the transition to a magnetically ordered phase.

We investigate the structure/property relationships in magnetocaloric compounds using macroscopic magnetization measurements, as well x-ray and neutron powder and single crystal diffraction. Our investigations concentrate on two systems. Compounds in the system $Mn_{5-x}Fe_xSi_3$ undergo a variety of phase transitions from paramagnetic to ferromagnetic or antiferromagnetic phases which are accompanied by a sizeable magnetocaloric effect [1,2]. Temperatures of the transitions vary depending on their iron content. In compounds of the system $Mn_{2-x}Co_xSb$, on the other hand, the magnetocaloric effect is associated to a ferrimagnetic to antiferromagnetic transition.

We will report on multiparametric studies of the compounds in both systems and discuss the influence of temperature, hydrostatic pressure and the variation of chemical composition on the magnetic transitions and the deformation of the crystal lattice. In addition, we will point out striking similarities in the behaviour of both systems which might serve to better define the basic structural requirements for magnetocaloric materials.

1. Songlin, et al., J. Alloys Comp. 334, 249-252 (2002).
2. P. Hering et.al., Chem. Materials 27, 7128-7136 (2015).

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