Mechanism of Magneto-structural transformation in Mn based Antiperovskites

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Abstract

One class of materials that has attracted attention as candidates for ferroic cooling applications are the Mn based antiperovskite materials (ABX_3). Amongst these $GaCMn_3$ undergoes a cubic-cubic volume discontinuous first order transition from a ferromagnetic (FM) to an antiferromagnetic (AFM) ground state at 160K [1] accompanied by a large and table like magnetocaloric effect in relatively low fields [2] and a recyclable adiabatic temperature change of 3K [3]. On the other hand, isostructural $SnCMn_3$ exhibits a sharp first order change from a paramagnetic (PM) state to a complex AFM and FM state at 279K accompanied by a conventional magnetic entropy change and negligible transitional hysteresis [4,5]. The solid solutions of these two compounds, although structurally single phase show a clear magnetic phase separation leading to frustrated magnetic ground states [6-8].Through a confluence of different techniques like x-ray, neutron diffraction and x-ray absorption fine structure (XAFS) spectroscopy we dissect the role of constituent atoms in the magneto-structural transition in these materials. It is shown that the local structural distortions introduced by the size and electronic configuration of A site atom plays an important role in the first order magneto-structural transition and associated magnetocaloric effect.

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