Anharmonic Lattice Effect in the Giant Negative Thermal Expansion Antiperovskite Cu$_{1-x}$Sn$_x$NMn$_3$  

PENG TONG, DESPINA LOUCA, Department of Physics, University of Virginia, GRAHAM KING, ANNA LLOBET, Los Alamos National Laboratory, BOSEN WANG, YUPING SUN, Institute of Solid State Physics, Chinese Academy of Sciences — The antiperovskite ANMn$_3$ (A: transitional metals and semiconducting elements) often shows a large, discontinuous volume contraction at the magnetic transition associated with a large negative thermal expansion (NTE). The NTE property was initially observed in Cu$_{1-x}$Ge$_x$NMn$_3$ where Ge-doping broadens the discontinuous volume contraction. It was recently reported that although the average symmetry is cubic in the solid solutions, locally, the symmetry is tetragonal with the I4/mcm symmetry of the end member GeNMn$_3$. We investigated the local structure of a “Ge”-free NTE system, the Cu$_{1-x}$Sn$_x$NMn$_3$ with $x = 0.1$ and 0.5. On average, both compounds are cubic at all temperatures. At base temperature, the local structure is cubic as well. As the temperature rises however, local lattice distortions evidenced by the splitting of the Mn-Cu and Mn-Sn bonds are observed. This local distortion can be described by the I4/mcm symmetry but this symmetry is different from the P4/mmm symmetry of SnNMn$_3$. The splitting of the Mn-Cu and Mn-Sn bond gives rise to a local lattice anharmonicity that may in turn be significant in the NTE behavior in this class of compounds.

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