Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Impact of electron doping on structure and dynamics of synthetic tetrahedrite[1] JENNIFER L. NIEDZIELA, ANDREW F. MAY, MICHAEL A. MCGUIRE, Oak Ridge National Laboratory, Materials Science Division, DOUGLAS L. ABERNATHY, Oak Ridge National Laboratory, Quantum Condensed Matter Division, MELANIE J. KIRKHAM, Oak Ridge National Laboratory, Instrument and Source Division, EDGAR LARA-CURZIO, OLIVIER DELAIRE, Oak Ridge National Laboratory, Materials Science Division — Microscopic control of lattice thermal conductivity is critical to the development of thermoelectric materials. One route to this control is manipulation of anharmonic lattice dynamics with chemical doping. Tetrahedrite compounds, which display an intrinsic lattice anharmonicity, are promising candidates for thermoelectric application, and here we present results of neutron scattering studies on synthetic $Cu_{12-x}Zn_xSb_4S_{13}$, ($x = 0,\ 2$). The undoped compound exhibits a structural phase transition associated with a metal-insulator transition near 88 K. Doping with Zn results in the stabilization of the structure, and enhancement of a low energy vibrational mode associated with incoherent oscillations of Cu. The low energy mode is localized, and exhibits pronounced softening with temperature. The ability to tune the location of this low-energy mode with doping may provide a means to enhance the phonon-phonon scattering that leads to low thermal conductivity in these materials, and a corresponding enhancement of the thermoelectric properties.

[1]This work was supported by the United States Department of Energy

Jennifer L. Niedziela
Oak Ridge National Laboratory, Materials Science Division

Date submitted: 06 Nov 2015 Electronic form version 1.4