Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Atomic Disorder in Tetrahedrite JOHN ROBERT SALASIN, Univ of Tennessee, Knoxville, BRYAN CHAKOUMAKOS, Oak Ridge National Lab, CLAUDIA RAWN, Univ of Tennessee, Knoxville, ANDREW MAY, EDGAR LARA-CURZIO, MICHAEL MCGUIRE, HUIBO CAO, Oak Ridge National Lab — Thermoelectrics (TE) are materials which turn heat energy into electrical energy with applications spanning multiple disciplines including space exploration, Peltier cooling, and engine efficiency. Tetrahedrite is a copper sulfosalt with the general formula $Cu_{12-x}M_x(Sb,As)_4S_{13}$. Where M denotes a Cu^{2+} site frequently replaced in natural tetrahedrite with Zn, Fe, Hg, or Mn. It has a cubic structure with an I-43m symmetry,a =10.4 Å, and only a handful of adjustable parameters. This structural study corroborates theoretical calculations on atomic disorder. Positional disorder of the trigonally coordinated Cu(2) site is suggested from the temperature dependence of the atomic displacement parameters determine from single-crystal x-ray and neutron diffraction.[1] The displacements are extremely anisotropic for Cu(2) with a maximum rms static displacement of $\sim$ 0.25 Å.

[1]This research at ORNL's High Flux Isotope Reactor and Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

John Robert Salasin
Univ of Tennessee, Knoxville

Date submitted: 14 Nov 2014 Electronic form version 1.4