Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Phonon self-energy and origin of anomalous neutron scattering spectra in SnTe and PbTe thermoelectrics[1] CHEN LI, Oak Ridge National Lab, OLLE HELLMAN, Department of Physics, Chemistry and Biology, Linköping University, JIE MA, ANDREW MAY, XIN CHEN, DAVID SINGH, BRIAN SALES, HUIBO CAO, ANDREW CHRISTIANSON, GEORG EHLERS, OLIVIER DELAIRE, Oak Ridge National Lab — The anharmonic lattice dynamics of rock-salt thermoelectric compounds SnTe and PbTe are investigated with inelastic neutron scattering and first-principles calculations. The experiments show that, surprisingly, although SnTe is closer to the ferroelectric instability, phonon spectra in PbTe show a more anharmonic character. This behavior is reproduced in first-principles calculations of the temperature-dependent phonon self-energy. Our simulations reveal how the nesting of phonon dispersions induces prominent features in the self-energy, which account for the measured energy spectra and their temperature dependence. The contributions to the complex features of the transverse-optic ferroelectric mode from phase-space for three-phonon scattering processes and the lattice instability are compared.

[1]We acknowledge funding from the US DOE, Office of Basic Energy Sciences, Materials Science and Engineering Division, and from the S3TEC Energy Frontier Research Center, DOE DE-SC0001299.

Chen Li
Oak Ridge National Lab

Date submitted: 14 Nov 2013 Electronic form version 1.4