Temperature Effects in Lattice Dynamics of SnSe

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Tinselenide demonstrates a record high thermoelectric figure of merit [1]. The distinctive feature of this material is very low thermal conductivity directly related to peculiarities of SnSe lattice dynamics. We studied the temperature dependence of the crystal structure, phonon dispersion curves and vibrational density of states (VDOS) of SnSe in the temperature range from 300 to 750 K using neutron scattering instruments at ANSTO. We found that frequencies of longitudinal and transverse phonons in SnSe have remarkably low frequencies, in particular the acoustic phonons propagating along *a* - axis perpendicular to the *b*-*c* layers. The low-energy TO_c[100] optic mode polarized along *c*-axis is highly anharmonic and shows the soft-mode behavior. Measurements of VDOS during heating reveal rather complex modifications of the spectrum showing a significant softening of SnSe phonon frequencies as a function of temperature. The DFT-MD simulation describes softening of phonons at frequencies around 7.5 and 16 meV in agreement with the experiment. By analyzing the displacements of a Sn atom from DFT-MD, the strong anisotropy of thermal parameters was found near the phase transition temperature.

[1] L. Zhao, et al., Nature, 508 (2014) 373