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Phonon dynamics in SnTe[1] CHEN LI, OLIVIER DELAIRE, XIN CHEN, DAVID SINGH, ANDREW MAY, JIE MA, MICHAEL MCGUIRE, GEORG EHLERS, ANDREW CHRISTIANSON, ASHFIA HUQ, Oak Ridge National Laboratory — Thermoelectric materials can convert waste heat into electrical energy, and have attracted much attention in recent years for power generation. IV-VI compounds in rock salt structure include some of the most efficient thermoelectric materials and giant phonon anharmonicity is believed to contribute to the low thermal conductivity. In this work, phonon dispersions and linewidths in single-crystalline SnTe were measured at a series of temperatures using time-of-flight and triple-axis neutron spectrometers to study the temperature dependence of the phonon dynamics and phonon anharmonicity. Phonon calculations and molecular dynamics simulations with first-principles methods were used to identify the anomalies in phonon modes and the results were compared to the measurements. Because the phonons involved have an important contribution to the lattice thermal conductivity in this system, the anharmonic coupling is likely to provide a key insight in understanding the surprisingly low thermal conductivity of the rocksalt tellurides in general.

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