

Abstract Submitted
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Phonon Density of States in Equilibrium and Non-equilibrium Prepared Ytterbium and Cerium-Filled Skutterudites IVO DIMITROV, Brookhaven National Laboratory, MICHAEL MANLEY, Lawrence Livermore National Laboratory, QING JIE, JUAN ZHOU, JORGE CAMACHO, Brookhaven National Laboratory, GEORG EHLERS, ANDREY PODLESNYAK, Oak Ridge National Laboratory, STEVEN SHAPIRO, QIANG LI, Brookhaven National Laboratory — Filled skutterudites have been extensively studied due to their high thermoelectric figure of merit (ZT) and promise for applications in the 400 K – 800 K range. They tend to exhibit higher ZT values than their binary counterparts, and a so-called “rattling effect” has been suggested to be a major factor that effectively reduces lattice thermal conductivity. However, this “rattling” scenario for the vibrational modes of a heavy element in a skutterudite cage remains controversial. We measured the phonon density of states (DOS) of Ce and Yb-filled skutterudites prepared by conventional equilibrium and non-equilibrium synthesis methods via inelastic neutron scattering. Nanoscaled substructures are commonly observed in the non-equilibrium samples as examined by high resolution TEM. Preliminary data analysis shows that the Yb filled antimonides exhibit well-defined localized modes in the 4-12 meV range and several unresolved optical modes in the 30-35 meV range, as compared with their Ce-filled counterparts. Differences in the 3-10 meV range in the DOS of the latter are believed to arise from non-equilibrium structures that developed during preparation.

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