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Crystal Structure Effects on the Thermal Conductivity of Cu-Ge-Se Compounds¹ ERIC SKOUG, JEFFREY CAIN, DONALD MORELLI, Michigan State University, MICHIGAN STATE UNIVERSITY TEAM — One approach to increasing the efficiency of a thermoelectric material is to decrease its thermal conductivity without degrading its electronic properties. Traditionally this has been accomplished, for instance, by forming solid solutions between compounds with similar crystal structures, or, more recently, by inducing nanostructure in the crystal lattice. These methods have proven effective in many cases; however discovering compounds with intrinsically low thermal conductivity provides a fundamental solution to the same problem. Here we describe our initial efforts in synthesis and characterization of compounds of the series $\text{Cu}_2\text{Ge}_{1+x}\text{Se}_3$, in which we observe a transition from orthorhombic to cubic symmetry at $x = 0.55$. The lattice thermal conductivity of the cubic phase is significantly lower than that of the orthorhombic phase, which we discuss here in relation to vacancies and anti-site defects. A simple valence argument is presented suggesting a change in the nominal valence of Ge as x approaches 1.0, which we speculate contributes to increased bond anharmonicity in the cubic-structure compounds.

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