

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**Anharmonic vibrational effects of thermoelectric Cu-Sb-Se ternary semiconductors: Density-functional theory studies** YONGSHENG ZHANG, Materials Science and Engineering, Northwestern University, ERIC SKOUG, JEFFREY CAIN, DONALD MORELLI, Chemical Engineering and Materials Science, Michigan State University, VIDVUDS OZOLINS, Materials Science and Engineering, University of California, Los Angeles, CHRISTOPHER WOLVERTON, Materials Science and Engineering, Northwestern University — Strong anharmonicity can lead to intrinsically minimal thermal conductivity even in defect-free single crystals. In an effort to understand this behavior, we have investigated two Cu-Sb-Se ternary semiconductors,  $\text{Cu}_3\text{SbSe}_4$  and  $\text{Cu}_3\text{SbSe}_3$ , by both experimental measurements and density functional theory (DFT) calculations. The experimental lattice thermal conductivity measurements show that while  $\text{Cu}_3\text{SbSe}_4$  exhibits classical behavior, the lattice thermal conductivity in  $\text{Cu}_3\text{SbSe}_3$  is anomalously low and nearly temperature independent. The vibrational properties of these two semiconductors are calculated by DFT phonon calculations within the quasi-harmonic approximation. The average of the Grüneisen parameters of the acoustic mode in  $\text{Cu}_3\text{SbSe}_3$  is larger than that of  $\text{Cu}_3\text{SbSe}_4$ , which theoretically confirms that  $\text{Cu}_3\text{SbSe}_3$  has a stronger lattice anharmonicity than  $\text{Cu}_3\text{SbSe}_4$ . Using our DFT-determined longitudinal and transverse Grüneisen parameters, Debye temperatures, and phonon velocities, we calculate the lattice thermal conductivity using the Debye-Callaway model (without the use of any adjustable parameters). The calculated thermal conductivity is in good agreement with the experimental measurements.

Yongsheng Zhang  
Materials Science & Engineering, Northwestern University

Date submitted: 07 Nov 2011

Electronic form version 1.4