

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**First-principles study of anharmonic lattice dynamics and thermal conductivity of AgSbTe<sub>2</sub>** YI ZHANG, Department of Physics and Astronomy and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, PAUL KENT, Computer Science and Mathematics Division, Oak Ridge National Laboratory, JIHUI YANG, Department of Materials Science and Engineering, University of Washington, CHANGFENG CHEN, Department of Physics and Astronomy and High Pressure Science and Engineering Center, University of Nevada, Las Vegas — We report on first-principles calculations of anharmonic lattice dynamics and thermal conductivity of AgSbTe<sub>2</sub>. We study the temperature dependence of phonon scattering and, in particular, examine the mechanism responsible for the low thermal conductivity of AgSbTe<sub>2</sub>, which holds the key to its potential thermoelectric applications. We perform systematic calculations and analysis to discuss the role of intrinsic anharmonic phonon-phonon scattering and strong phonon-nanodomain scattering in determining the phonon transport process in AgSbTe<sub>2</sub>.

Yi Zhang  
Univ of Nevada - Las Vegas

Date submitted: 15 Nov 2013

Electronic form version 1.4