Phonon Mean Free Path Distribution of Bi_2Te_3: a Comparison Between Thermal Measurements of Thin Films and First-Principles Calculations

Xiaowei Lu
Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China

Sien Wang [S]
Department of Aerospace and Mechanical Engineering, University of Arizona, Tucson, Arizona, U.S.A.

Ankit Negi
Department of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, North Carolina, U.S.A.

Hezhu Shao
College of Electrical and Electronic Engineering, Wenzhou University, Wenzhou, China

Peng Jiang
Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China

Jun Liu
Department of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, North Carolina, U.S.A.

Qing Hao [C]
Department of Aerospace and Mechanical Engineering, University of Arizona, Tucson, Arizona, U.S.A.
qinghao@arizona.edu

There has been a growing interest in solid-state thermoelectric (TE) materials for their applications in energy conversion and harvesting. As a dimensionless parameter commonly used to assess the efficiency for TE energy conversion, the TE figure of merit (ZT) can be improved by reducing the thermal conductivity of the material, while keeping bulk-like electrical properties. This can be achieved by introducing nano-sized structures to suppress the phonon transport. Knowledge of spectral phonon mean free paths is critical for evaluating the thermal conductivity reduction using above classical phonon size effects. Nanostructured bismuth telluride (Bi_2Te_3) has shown considerable improvements in the ZT value. However, the anisotropic thermal conductivity in crystalline Bi_2Te_3 is still not well understood due the challenge in preparing high-quality single crystals for accurate thermal measurements. In this regard, the present work aims at understanding the room-temperature thermal transport in Bi_2Te_3 thin films along the in-plane and cross-plane directions. High-quality Bi_2Te_3 thin films have been prepared using chemical vapor deposition on a SiO_2/Si substrate. Thickness-dependent thermal conductivity has been measured along the cross-plane direction and compared to the predictions based on first-principles-calculated spectral phonon mean free paths in the bulk material. The film thickness ranges from 20 nm to 300 nm, as confirmed using the atomic force microscopy. Time domain thermoreflectance (TDTR) experiments have been performed at two different modulation frequencies to decouple the effect of the interfacial conductance. The measured room-temperature thermal conductivity has a weak dependence on the film thickness, suggesting that mean free path of most phonons is smaller than 20 nm. The in-plane phonon mean free path distribution is also computed. Literature data for various nanostructured Bi_2Te_3 are re-analyzed based on these phonon mean free path distributions. This result could provide important guidance for ZT enhancement within nanostructured Bi_2Te_3 alloys.