Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Computational study of phonon scattering induced by dislocations BEN XU, YANDONG SUN, Tsinghua university, YANGUANG ZHOU, MING HU, RWTH-AACHEN, YUANHUA LIN, Tsinghua university — Recent experiments showed dislocation-phonon interaction is important to enhance thermoelectric properties of materials. But the basic understanding of this interaction is far from satisfactory. Here, thermal conductance and phonon spectrum are carried out computationally for sample with dislocations, particularly for materials Fe and PbTe, attributed to the core and strain field of the dislocation. We find that the scattering is not limited to the traditional high frequency, but also is significant to phonon with medium frequency. Moreover, detailed analysis demonstrates how the dislocation interact with the eigen vibration mode of the material.

Ben Xu
Tsinghua university

Date submitted: 04 Jan 2017 Electronic form version 1.4