Modeling Thermal Transport in Realistic Nanostructured Materials

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Thermal conductivity (κ) of crystal nanostructured semiconductors is dominated by phonons, which are lattice vibrations that can be quantized as quasiparticles having mean free paths (MFPs). The behavior of these particle-like phonons can be modeled by the Peierls Boltzmann transport equation (BTE) [1]. The linearized form of the Peierls BTE can be solved approximately by using the Monte Carlo ray-tracing (MCRT) technique, with intrinsic phonon properties from the first-principles-based lattice dynamics, and the specularity and transmittance at the interfaces from the diffusive mismatch model (DMM) or atomistic Green's function calculation, as has been illustrated in the previous works [2, 3].

Here, we further demonstrate that the MCRT method could be an effective way of modeling phonon transport in realistic nanostructured materials. Two polycrystal graphite specimens with average grain sizes of 2.75 micrometers and 5.3 micrometers were employed as the typical examples for the investigation. The nanostructures in our simulation are constructed exactly based on the scanning electron microscope (SEM) image of the specimens (Fig. 1(a)). Periodic conditions are applied to the system in y and z directions. Specularity and transmittance at the interfaces between the grains are set according to the DMM. Bulk phonon properties of graphite are obtained by solving the BTE using the iterative method [4] with interatomic forces constants from first-principles (FP). Fig. 1(b) shows the agreement of the predicted κ of the graphite specimens and experiment measurements at 300 K, which validates our calculations. In the presentation, we will also discuss the effect of local the transmittance of each interface on κ and temperature dependence of κ.

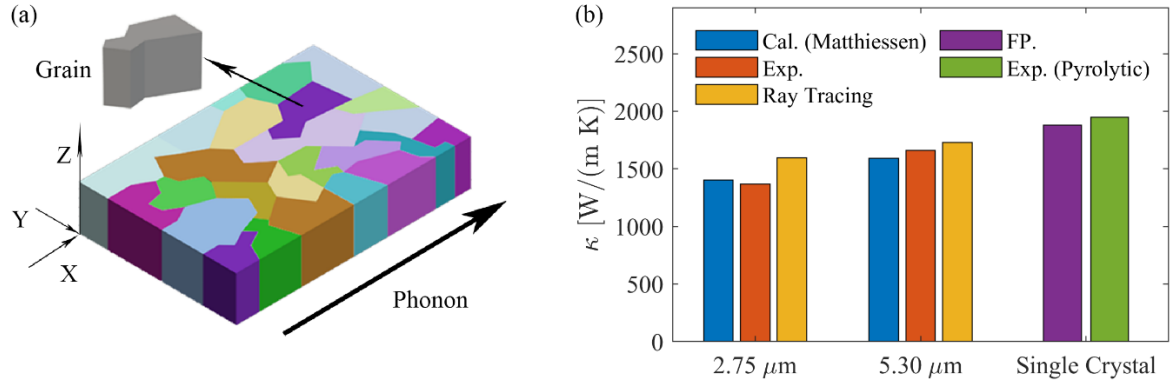

Fig. 1 Structures of graphite constructed from SEM image (a) and a comparison of the calculated κ with measured values (b). The calculated values are obtained using Matthiessen's rule [3] and experimental data of pyrolytic graphite is from the work of Ho *et. al.* [5]

Reference

[1] R. Peierls, Annalen der Physik (1929). [2] T. Hori, Appl Phys Lett (2015). [3] T. Oyake, Phys Rev Lett (2018). [4] W. Li, Comput Phys Commun (2014). [5] C. Y. Ho, J Phys Chem (1972)