Cross Plane Heat Transport Across the 2D/3D Material Interfaces

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Abstract

Understanding the heat transport in two-dimensional (2D) materials is necessary for the reliable operation and performance of the devices made from these materials. When the device sizes decrease, the interfaces between the 2D materials and their substrates contribute more to the thermal transport mechanisms. As a result, thermal boundary conductance (TBC) that defines the thermal transport rate at the interfaces becomes a key parameter for the thermal characterization and design of 2D devices. In this study, we perform approach – to – equilibrium molecular dynamics simulations to evaluate the TBC of interfaces between popular 2D materials (h-BN, MoS_2, WS_2, WSe_2) and substrates (GaN and SiO_2) Simulation results are used to calculate the lattice vibration (i.e. phonon) properties of the materials using a new approach based on the fluctuation-dissipation theorem and atomistic Green's functions. Our results suggest that the TBC of the interfaces mostly depend on the similarities and the differences between the lattice vibrational properties of the materials making the interface. Moreover, the number of 2D material layers and the lattice match between the 2D and substrate materials also affect the TBC. The results of the simulations are used to generate a correlation to calculate the TBC of the interfaces based on a function, *I*, that depends on the materials' phonon dispersions, temperature, mass ratio of atoms, and number of 2D material layers. These findings are also compatible with the existing TBC data in the literature [1-3]. We believe the correlation obtained in this study will be a good guide for the selection of the thermally superior substrates for 2D-based applications.

References

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Figures

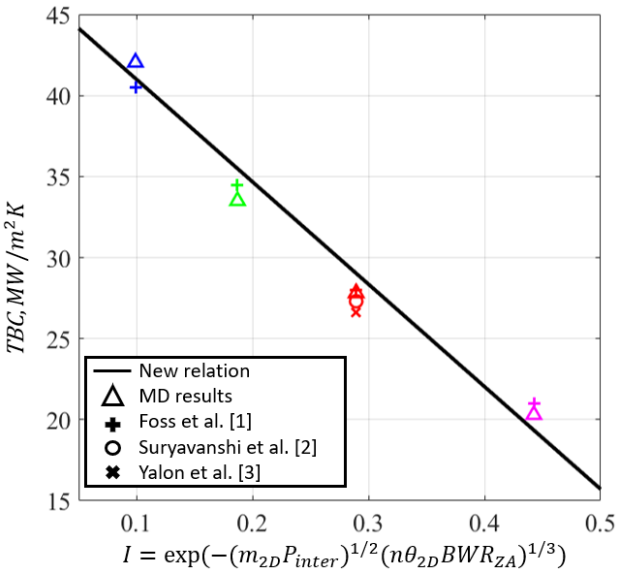

Figure 1: Comparison of the proposed model, MD results of this study, and the results from the literature [1-3].