Thermal Effects in Two-Dimensional Materials: The Role of 2D/3D Interfaces

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Two-dimensional (2D) materials have tremendous potential for next-generation nano- and optoelectronics. However, heat dissipation and its removal from hot spots in the monolayer remains a critical concern to the design of 2D-based devices [1]. Thermal currents flowing in an atomic layer can either dissipate through source/drain contacts in a transistor configuration, or through a supporting substrate via van der Waals (vdW) coupling to it. When a 2D material is supported by a substrate, the interfacial area formed between it and the substrate is often far larger than the lateral source/drain contact area. Thus, the majority of waste heat is removed across the 2D-substrate interface and then via the substrate. The thermal boundary conductance (TBC) between the 2D layer and substrate should be well characterized for reliable 2D device performance. Interfaces formed between 2D vdW materials and 3D substrates are fundamentally different than same-dimension 3D-3D and 2D-2D interfaces due to the presence of a vdW gap and the different dimensionalities of the phase spaces on either side of the interface. In this invited talk, I will review the progress in understanding lattice thermal transport, both in-plane and cross-plane, in 2D mono and few-layer materials. Then I will introduce my recent work aimed to tackle the question of selecting the best substrate for each 2D material from the point of view of heat dissipation.

Several recent papers measured the TBC between various monolayers and mostly the silicon dioxide (SiO_2) substrate, reporting a wide range of values due to inconsistent sample quality. Therefore, it is imperative to build predictive methods for quantifying the TBC between MLs and various substrates. Here, we use a combination of phonon dispersions from first-principles density functional perturbation theory simulations and our 2D-3D TBC model [2, 3]. We investigate the TBC between combinations of six atomic layers (h-BN, graphene, MoS_2, $MoSe_2$, WS_2, and WSe_2) and six substrates (SiO_2, AlN, GaN, 6H-SiC, diamond, and Al_2O_3). We show that TBC is higher for softer substrates with smaller speed of sound, but of the 6 substrates we compared, amorphous SiO_2 consistently produced higher TBC than crystalline substrates. Our work helps build a roadmap for quantifying the TBC between various 2D monolayers and their substrates and provides a framework for other 2D-3D interfaces to be studied.

[1] Yalon, E., et al., *Nano Letters* **17**(6), 3429–3433 (2017).

[2] Yasaei, P., et al., *Advanced Materials Interfaces* , 1700334 (2017).

[3] Correa, G. C., Foss, C. J., and Aksamija, Z. *Nanotechnology* **28**(13), 135402 (2017).

Phonon Thermal Transport in Nanostructured Materials

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The management of heat and the understanding of heat transfer are ubiquitous challenges in numerous sciences and technologies, from models of Earth's thermal history to managing local hot spots in microelectronics. Computational materials physics is now playing an increasingly important role in developing fundamental insights into the lattice thermal conductivity of solids, a fundamentally important parameter that determines the utility of a material for energy-related applications including thermoelectricity, heat dissipation and manipulation, and thermal analogs to electronic components (e.g., thermal diodes and switches).

Here I will discuss a *predictive* method for modeling lattice dynamical properties and thermal conductivity: Peierls-Boltzmann transport coupled with density functional theory. Focus will be given to application of this method to nanostructured materials (e.g., 2D and layered vdW bonded systems, 1D chains), particularly as symmetry and dimensionality govern phonon interactions and transport. I will discuss phonon chirality and symmetry-based phonon scattering rules in 1D chains, invariance conditions for 2D materials, and the influence of anisotropy in bulk hBN and MoS_2.

This work was supported by the Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.