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Thermal boundary conductance of beyond graphene two-dimensional materials CAMERON FOSS, ZLATAN AKSAMIJA, Univ of Mass - Amherst — An ongoing concern for 2D materials is their ability to thermally couple with their underlying substrate which acts as the primary pathway for heat removal in 2D devices. The thermal pathway from the 2D layer to substrate has been studied rigorously in graphene and various transition metal dichalcogenides. However, the literature still lacks a comprehensive analysis of thermal boundary conductance (TBC) for beyond-graphene materials. Previously [2D Mater. 6 (2019) 025019] we have shown that the TBC depends strongly on the overlap of available phonon modes in the long-wavelength regime and found selection criteria for choosing the best substrate for TBC. Here we use a combination of first-principles calculations and phonon interface transport modeling to calculate the TBC of several beyond-graphene 2D materials, such as; silicene, germanene, stanene, BAs, GaAs, InAs, and blue and black phosphorene, on amorphous and crystalline substrates. Our results show the TBC for these 2D materials on amorphous SiO_2 (a-SiO_2) falls between 20-50 $MW.m^{-2}.K^{-1}$, with the highest TBC being found in BAs due to its extremely flat ZA branch lending to a large low-energy density of states. A trend emerges that 2D materials with lower ZA branch frequencies have higher TBCs when placed on a-SiO_2. Our results provide selection criteria for 2D materials that improve interfacial heat transport in 2D devices with amorphous and crystalline substrates.

Cameron Foss
Univ of Mass - Amherst

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