Thermal properties of novel 2D hybrid graphene-BN nanostructures

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— Graphene, a 2D honeycomb carbon crystal of one-atom thickness, has been widely recognized as a very promising material for next generation optoelectronic and NEMS applications. Recent developments have shown that it is possible to obtain hybrid 2D structures by combining sp2-graphene lattice with sp2-lattice of non-carbon materials such as hexagonal Boron Nitrides. The atomically thin sheets containing both hexagonal-Boron Nitride and graphene can result in new materials with properties complementary to their individual properties and further enrich the potential applications. Here, using molecular dynamics simulations, we elucidate the characteristics of thermal transport in 2D hybrid h-BN and graphene materials. We find the thermal conductivity of the hybrid material is a strong function of the relative domain widths, interface type (e.g., zigzag and armchair) as well as the interface quality. Our results provide crucial insights on the role of the interfaces and defects in phonon scattering in the hybrid material and can potentially provide means to tailor its thermal properties.