Disorder Enhanced Thermal Conductivity Anisotropy in Two-Dimensional Materials and van der Waals Heterostructures

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Two-dimensional (2D) materials and van der Waals heterostructures can naturally function as directional heat spreaders in nanoelectronics due to their intrinsically anisotropic structure. In the real nanoelectronics applications, disorders usually appear in those materials where their effects on anisotropic thermal conductivity are not well-understood. We built simple graphite-like materials models and systematically incorporated mass disorder or structural disorder into the structures. The anisotropic thermal conductivities calculated by equilibrium molecular dynamics simulations show that mass disorder and stacking disorder can effectively and anisotropically tune the thermal conductivity of 2D materials and van der Waals heterostructures. Compared with the pristine graphite, the through-plane thermal conductivity can be reduced up to two orders of magnitude by the through-plane mass disorder and the thermal anisotropy ratio (i.e., the ratio of in-plane to through-plane thermal conductivity) can be enhanced more than ten times. We attribute this counter-intuitive result to the dramatic decrease of phonon group velocity in the through-plane direction. Our results can shed some lights on the thermal management in electronics incorporating 2D materials and van der Waals heterostructures.