Molecular Dynamics Simulations of the Thermal Conductivity of Layered Materials: Crossover from In-Plane to Cross-Plane

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Molecular dynamics simulations have been widely used to calculate the thermal conductivity of nanostructures. One type of structure of great potential for photovoltaic, thermoelectric, thermal insulation, and heat dissipation applications is the layered material. Previous studies on the thermal transport in layered materials focused on either the in-plane or the cross-plane direction. Here we use nonequilibrium molecular dynamics simulations to study the crossover from in-plane to cross-plane thermal transport, by considering model systems made of silicon and germanium and incorporating novel geometrical designs. We find that (1) the thermal conductivity decreases gradually as the thermal transport changes from in-plane to cross-plane, (2) the thermal conductivity increases as the thickness of the interfacial region increases (due to a phonon bridging effect), and (3) the conventional serial and parallel thermal resistance models for layered materials provide deviated predictions when the neighboring layers have strong interactions with each other. This study is potentially useful for tuning the thermal conductivity of layered nanostructures for the relevant applications.