Aperiodic van der Waals heterostructures with minimum thermal conductivity

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Van der Waals (vdW) heterostructures vertically stacked from isolated two-dimensional atomic layers have triggered tremendous attention due to their promising applications in electronic devices including tunneling transistors, barristors and flexible electronics, as well as optoelectronic devices.[1] Thermal transport in the stacking direction of these heterostructures plays a pivotal role in determining their thermal properties and performance. Here, we perform materials informatics to explore the controllability of thermal transport in vdW graphene-MoS_2 and graphene-WS_2 heterostructure thin films and identify the ultimate heterostructure that gives minimum thermal conductivity, respectively. The thermal conductivities of heterostructures with different stacking order are calculated from the non-equilibrium molecular dynamics simulation, and the black-box optimization is conducted by coupling it with machine learning, namely Bayesian optimization that can realize highly efficient optimization [2-3].

The identified optimal graphene-MoS_2 heterostructures are aperiodic but non-random and exhibit significantly lower thermal conductivity compared with periodic counterparts as shown in Fig. 1. Prior to the optimization of graphene-WS_2 heterostructure, effect of area (cross-sectional area perpendicular to the direction of heat flow) on thermal conductivity of WS_2, graphene and graphene-WS_2 superlattice is studied as shown in Fig. 2. Thermal conductivity of WS_2 and graphene-WS_2 superlattice is lower than that of MoS_2 and graphene-MoS_2 superlattice, which is reasonable considering the mismatch in the mass density and phonon density of states. Moreover, the mechanism of the reduction is further studied in terms of distributions of spectral phonon transmissions and eigenmodes, and the results help characterizing the localization of coherent phonons, where the transmissions distribution suggest Anderson type but the superiority of specific non-random structure suggests contribution of Fabry Perot type. This research deepens our understanding of the thermal transport of van der Waals heterostructures and provides guidance for the design and control of their thermal properties.

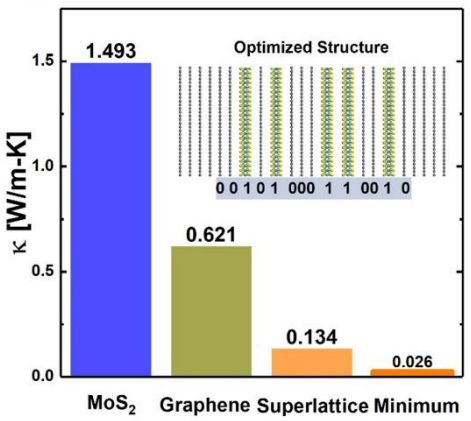

Fig. 1 Comparison of the thermal conductivity

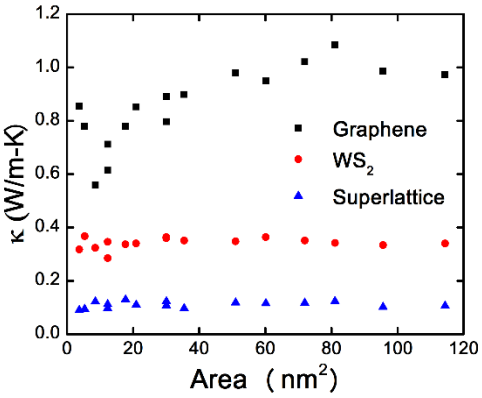

Fig. 2 Thermal conductivity with increase of area

References

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