Hexagonal Boron Nitride: A Promising Substrate for Graphene with High Heat Dissipation

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Abstract

Supported graphene on standard SiO_2 substrate exhibits unsatisfactory heat dissipation performance that is far inferior to the intrinsic ultrahigh thermal conductivity of the suspended sample. A suitable substrate for enhancing the thermal transport in the supported graphene is highly desirable to the development of graphene devices for thermal management. By using the molecular dynamics simulations, here we demonstrate the bulk hexagonal boron nitride (*h*-BN) is a more appealing substrate to achieve high performance heat dissipation in supported graphene. Notable length dependence and high thermal conductivity are observed in *h*-BN supported SLG, suggesting that the thermal transport characteristics are close to that in the suspended SLG. At room temperature, thermal conductivity of *h*-BN supported SLG is as high as 1347.3±20.5 $Wm^{-1}K^{-1}$, which is about 77% of that for the suspended case and is more than twice of that for the SiO_2 supported SLG. Furthermore, we find the smooth and atomically flat *h*-BN substrate gives rise to the regular and weak stress distribution in graphene, resulting in the less affected phonon relaxation time and dominant phonon mean free path. We also find stacking and rotation have significant impacts on the thermal transport in *h*-BN supported graphene. Our study provides valuable insights towards the design of graphene devices on realistic substrate for high performance heat dissipation applications.

Keywords: graphene; hexagonal boron nitride; substrate; thermal conductivity; heat dissipation; molecular dynamics