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Hexagonal Boron Nitride: A Promising Substrate for Graphene with High Heat Dissipation[1] ZHONGWEI ZHANG, SHIQIAN HU, JIE CHEN, Tongji Univ, BAOWEN LI, Colorado Univ — Supported graphene on standard SiO_2 substrate exhibits unsatisfactory heat dissipation performance that is far inferior to the ultrahigh thermal conductivity of suspended case. A suitable substrate for enhancing the thermal transport in supported graphene is highly desirable. By using molecular dynamics simulations, we have studied thermal conductivity of singlayer graphene (SLG) supported on bulk hexagonal boron nitride (h-BN) substrate. Notable length dependence and high thermal conductivity are observed in h-BN supported SLG, suggesting thermal transport properties are close to that in suspended SLG. At room temperature, thermal conductivity of h-BN supported SLG is as high as 1347.320.5 W/mK, which is about 77% of suspended case and more than twice of SiO_2 supported SLG. Furthermore, the h-BN substrate gives rise to a regular and weak stress distribution in graphene, which results in less suppressed phonon relaxation time and phonon mean free path. We also find stacking and rotation have significant impacts on structure dynamics and thermal conductivity of h-BN supported graphene. Our study provides valuable insights towards the design of realistic supported graphene devices with high performance heat dissipation.

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