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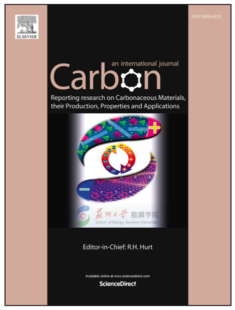

Substrate effects on the thermal performance of in-plane graphene/ hexagonal boron nitride heterostructures

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Substrate effects on the thermal performance of in-plane graphene/ hexagonal boron nitride heterostructures

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ABSTRACT

Interfacial thermal conductance *G* and effective thermal conductivity *k* of both freestanding and silica supported in-plane graphene/hexagonal boron nitride (Gr/h-BN) heterostructures are investigated via molecular dynamics simulations. The predicted *G* values (~10^{10} $Wm^{-2}K^{-1}$) are 3-4 orders larger than that of the van der Waals interfaces. Thermal rectification is found in such Gr/h-BN heterostructures for both freestanding and supported ones due to the mismatch of phonon spectra interrelated with temperature. Compared to the freestanding Gr/h-BN, an enhancement in the interfacial thermal transport is observed in supported ones and *G* becomes larger with increased substrate coupling. The calculated *k* is about 116-130 $Wm^{-1}K^{-1}$ for both freestanding and supported Gr/h-BN heterostructures in the temperature range from 200 to 600 K. A weaker temperature dependence is found in the *k* values compared with that of *G*, which is resulted from the inconsistent variation of thermal transport in single materials and across the interface with temperature. Our study offers perspectives of modulating thermal properties of two-dimensional heterostructures through surface interactions with the substrate, which can contribute to promoting its potential applications.

Keywords: Graphene; Hexagonal boron nitride; Two-dimensional heterostructures; Interfacial thermal conductance; Molecular dynamics

1. Introduction

The integration of two-dimensional (2D) materials into nanodevices has recently

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