Interfacial thermal resistance of 2D and 1D carbon/hexagonal boron nitride van der Waals heterostructures

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ABSTRACT

The newly emerging graphene/hexagonal boron nitride (h-BN) van der Waals heterostructures has attracted much research interest due to its new properties and functions for practical applications in nanodevices. In this work, molecular dynamics simulations are performed to study the interfacial thermal resistance (ITR) of a graphene/h-BN bilayer system as well as its one-dimensional counterpart, a concentric CNT/BNNT double-walled nanotube, based on the lumped capacity model. The calculated ITR is in an order of magnitude of 10^{-7} - 10^{-6} Km^2/W and it monotonically decreases with temperature and interlayer/intertube coupling strength. It is believed that the ITR between graphene and h-BN is reduced through the enhancement of the coupling strength instead of the geometrical overlap of the phonon modes. Heat flux direction has no effect on the ITR of the graphene/h-BN bilayer, however, radial thermal rectification is found in the CNT/BNNT composite, with a largest thermal rectification factor of $\sim 90\%$. Thermal energy always prefers to transport from the outer nanotube towards the inner nanotube in the CNT/BNNT system over the opposite direction no matter the outer nanotube is CNT or BNNT because the outer nanotube has more high-frequency phonons than that of the inner nanotube in the CNT/BNNT system.

1. Introduction

Following the tremendous research interests on graphene, the most representative two dimensional (2D) atomic crystal, with exceptional electronic, thermal, optical, magnetic and mechanical properties, other kinds of graphene-like 2D nanomaterials (such as h-BN, MoS_2 , WSe_2 and etc.) have also been intensively investigated in recent years due to their promising properties and a broad range of applications [1-3]. When

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these isolated monolayers or few-layer crystals are stacked layer by layer to ensemble a hybrid nanostructure, called van der Waals (vdW) heterostructure, it possesses the advantages of its individual components, and at the same time may exhibit new properties and functions for practical applications [4,5]. Nanoheterostructures composed of graphene and h-BN sheet [6], which has 2D sp^2 honeycomb structure and a crystal constant similar to that of graphene, have attracted much attention due to the unique and fascinating physical phenomena. The cone-shaped valence and conduction bands of graphene touch each other at the corners of the Brillouin zone, making it semimetallic while h-BN is a wide band gap insulator.

It is found that the band gaps and magnetic moments of bilayer or sandwich structured graphene/h-BN vdW heterostructures are tunable by external electric fields or strains [7-12], which enable the use of the heterostructures in electronics, spintronics, pressure sensors and etc. Lee et al. [13] prepared a tunneling rectifier from vertically stacked 2D materials composed of chemically doped graphene electrodes and h-BN tunneling barrier, which shows excellent diode performances and great potential for future flexible and transparent electronic devices. Chen et al. [14] measured a Seebeck coefficient of $-99.3 \mu\text{V/K}$ of the graphene/h-BN/graphene heterostructure device using an AC lock-in technique. Park et al. [15] revealed that an h-BN layer with some vacancies or metal impurities enhances the interlayer coupling in the graphene/h-BN heterostructure with respect to charge doping and electron scattering. Kim et al. [16] fabricated graphene field-effect transistors (FETs) with carbon channel placing directly on h-BN and SiO_2 . Small-signal transconductance and effective carrier mobility are improved by 8.5 and 4 times on h-BN, respectively, as compared with that on SiO_2 , which show potential of employing h-BN as a platform materials for large-area carbon electronics.

Despite of great efforts in theoretical and experimental explorations of graphene/h-BN vdW heterostructures, most of which are focused on its electronic and magnetic properties, thermal properties have not received significant attention so far. As the size of electronic devices continues scaling down, the effectiveness of heat

dissipation becomes a critical and urgent problem which limits the applications of the device. In nanoelectronics, thermal energies transport in a ballistic way when its feature size are comparable to the phonon mean free path. Interfacial thermal resistance (ITR) is an important physical quantity to characterize thermal properties of the system as well as thermal conductivity. In this work, we perform a molecular dynamics (MD) simulation to calculate the ITR of a graphene/h-BN bilayer system as well as its one-dimensional (1D) counterpart, a concentric CNT/BNNT [17] double-walled nanotube (DWNT), based on the lumped capacity model. Coaxial CNT/BNNT multi-walled structures are ideal components in nanoelectronic systems and separate CNTs and BNNTs can self-assemble into stable coaxial structures in water under appropriate condition [18]. The conductivity of the CNT core and the insulation of the BNNT sheath are found to be an ideal nanocable which owns light weight for suspending in nano-electro-mechanical system (NEMS) and high strength to resist the mechanical deformation [19]. So far, the thermal properties of the CNT/BNNT hybrid structures have not been reported. Results in this work provide fundamental knowledge for the applications of 1D and 2D C/h-BN vdW heterostructures in phonon engineering and nanoelectronics.

2. Modeling and Methods

The graphene is stacked 3.4 Å above the h-BN monolayer to model the 2D vdW heterostructure as depicted in Fig. 1(a). The AB configuration with one C atom directly above the B atom has been proven to be the lowest energy structure for the bilayer system [20-23]. The simulated bilayer nanoribbon is about $21.75 \times 2.51 \text{ nm}^2$. Fig. 1(b) and (c) show the atomic structures of two 1D CNT/BNNT composites, both with a favorable intertube distance of 3.4 Å [17,19]. The bond lengths of C-C and B-N are both 1.42 Å in the simulation with a lattice mismatch of $\sim 2.1\%$ for h-BN, which has negligible effects on its thermal properties [24,25]. The simulated 2D and 1D system are the same in length and consist of 4000 atoms and 4200 atoms, respectively. Therefore, the results of 2D and 1D system are comparable.

Fig. 1 - Atomic configuration of the C/h-BN heterostructures: (a) 2D system consisting of a graphene monolayer and an h-BN monolayer, (b) 1D DWNT with a (6, 0) CNT inside a (15, 0) BNNT, and (c) 1D DWNT with a (6, 0) BNNT inside a (15, 0) CNT. The pink, gray and blue balls represent B, C and N atoms, respectively.

The MD simulations are performed using the package LAMMPS and the Tersoff [26] potential is employed to describe the interactions among C-C atoms and B-N atoms, which has been used in numerous studies of the thermodynamics properties of C and BN low-dimensional nanostructures [27-32]. The C-BN couplings between the layers (2D) and the tubes (1D) are modeled as vdW interactions using Lennard-Jones (LJ) potential:

$$V(r) = 4\mu\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right] \quad (1)$$

Where σ is the equilibrium separation, ε is the well depth, and r is the distance between a pair of atoms to be considered. Parameter μ is used to adjust the interaction strength between C-BN atoms. The LJ parameters are $\varepsilon_{C-B} = 3.294$ meV, $\sigma_{C-B} = 3.411$ Å, $\varepsilon_{C-N} = 4.068$ meV and $\sigma_{C-N} = 3.367$ Å [33,34]. An integration time step of 0.4 fs is used and periodic boundary conditions are applied in the three directions with vacuum slabs large enough in the out-of-plane direction for the 2D system and in the radial direction for the 1D system to eliminate the effects of neighboring atoms.

To calculate ITR, the lumped capacity method is applied, usually used for calculating the Kapitza resistance [35,36]:

$$R = A\tau / C \quad (2)$$

where A is the interfacial area available for heat transfer, τ is the thermal relaxation time and C is the heat capacity of the system. It is necessary to assess the applicability of the lumped capacity method by using the Biot number, defined as

$$Bi = hL / k \quad (3)$$

where h is the thermal conductance (equal to inverse of the ITR), L is the distance through which heat is transferred, and k is the thermal conductivity of the C system or BN system in this case. The lumped capacity model can be used when $Bi < 0.1$. In the case of a bilayer system, for example, we calculated the in-plane thermal conductivity of the individual graphene nanoribbon and h-BN nanoribbon via non-equilibrium MD (NEMD) simulations, and it is 595 W/m/K and 330 W/m/K at 300 K for graphene and h-BN, respectively. To estimate the largest value of Biot number, we take the smaller value of the thermal conductivity of the monolayers, so $k = 330$ W/m/K is used. The interfacial conductance between graphene and h-BN is in an order of magnitude of 10^6 W/m²/K in previous studies [37,38] and $h = 1.0 \times 10^7$ W/m²/K is used here. Taking interlayer distance $L = 0.34$ nm, the largest value of Biot number is estimated to be 1.03×10^{-5} , well below the value of 0.1.

To obtain the time constant τ , for the first 200 ps within the NVT ensemble, C atoms and BN atoms are heated to (T+100) K and (T-100) K, respectively, and then reach the equilibration state. For the next 800 ps, the system relaxes under the NVE ensemble during which heat flows from the hot C system to the cold BN system and finally both the C system and the BN system reach about the equilibrated temperature T . Temperature of the C system and the BN system are recorded as a function of time every 1000 time steps, as exemplified in Fig. 2. From 200 ps to 1000 ps, the temperature difference ΔT , between the C system and the BN system, is fitted with the decaying exponential function as

$$\Delta T(t) = \Delta T(t=0) \exp(-t / \tau) \quad (4)$$

The heat capacity C of the isolated C system and BN system are calculated via independent simulations within the NVT ensemble from 200 K to 600 K for 400 ps and the total energy of the system is recorded as a function of temperature every 10000 time steps. The calculated total energy is linearly related with temperature and C is calculated via

$$C = dE / dt \quad (5)$$

where E is the total energy of the independent C or BN system. The heat capacity of the hybrid system is then calculated via

$$\frac{1}{C} = \frac{1}{C_C} + \frac{1}{C_{BN}} \quad (6)$$

where C_C and C_{BN} represent the heat capacity of C system and BN system, respectively.

Fig. 2 - Temperature evolutions of graphene, h-BN and the hybrid system within a NVT ensemble for 200 ps and a NVE ensemble for the next 800 ps. The exampled equilibration temperature is 300 K.

3. Results and Discussions

Fig. 3 shows the ITR of the 2D vdW heterostructure with different LJ scaling parameters, heat flux directions and temperatures ranging from 200 K to 600 K. The calculated ITR has an order of magnitude of 10^{-7} Km²/W, it decreases with temperature and interlayer coupling strength, and heat flux direction almost has no influence on the ITR of the bilayer system. Our results are consistent well with previous works. Zhang et al. [37] applied a transient MD simulation approach to the

graphene/h-BN bilayer system to investigate thermal transport across the layers and the calculated ITR is also in an order of magnitude of 10^{-7} Km²/W although the potential parameters and method are different from ours. By using Raman spectroscopy technique, Chen et al. [38] measured the thermal interface conductance of a graphene/h-BN junction with a value of 7.4×10^6 W/m²/K. In addition, the ITR in a bilayer system is larger than that in a heterostructure of multilayer graphene on h-BN substrate ($\sim 10^{-9}$ Km²/W), which indicates the interlayer coupling among multilayer graphene facilitates phonons to transmit through the heterojunction with the h-BN substrate [39].

Fig. 3 - ITR of a bilayer system composed of a monolayer graphene and a monolayer h-BN at different temperatures, LJ parameters and heat flux directions. C-BN and BN-C represent heat flux flows from graphene to h-BN and from h-BN to graphene, respectively.

The temperature dependence of ITR is attributed to the inelastic scattering of phonons at the interface [40] and the thermal relaxation time of phonons becomes smaller at a high temperature. When temperature increases, inelastic scattering which provides the major contribution to energy transport across the interface is supposed to be strengthened considerably and as a result the ITR drops obviously. Zhang et al. [37] believe that as the system temperature increases, more high frequency phonons will become activated and start making contribution to the interfacial thermal transport.

The influence of coupling strength on the heat performance at the interface has also been reported by Ong et al. [40,41], who investigated the thermal boundary

conductance between CNT and SiO₂ and the effects of substrate modes on the thermal transport in supported graphene and suggested that one may be able to control thermal transport in low-dimensional structures by modulating their coupling to substrates. To explain the underlying mechanisms of the influence of interlayer coupling strength on the ITR, the phonon density of states (DOS) that describes the distribution of vibration power at different frequencies is calculated, which is obtained from the Fourier transform of the velocity autocorrelation function [42]. Fig. 4 is the phonon DOS of the 2D system for different interlayer coupling strength at a temperature of 300 K. The overlapped areas of DOS, or the shared phonons region, is supposed to determine the amount of energy transported across the interface [43]. However, the overlapped areas of the phonon power spectrum remain unchanged with stronger coupling strength between the two monolayers although the ITR is reduced in this work. Xu et al. [44] summarized the possible improvements through nanoengineering the interfaces between CNTs. Besides the concept to select CNTs with similar structure or interfacial materials with a similar phonon spectrum to increase the phonon spectrum matching, the heat transfer performance can be improved by increasing the overlap length between CNTs to enlarge the geometrical overlap of phonon modes, or by introducing polymer wrapping or metal coating to enhance the coupling strength. Effective approaches to increase interfacial coupling include both the enlargement of geometrical overlap of phonon modes and the enhancement of interfacial coupling strength as Fig. 6 of [44] indicated. Therefore, the ITR of graphene/h-BN 2D system is reduced only through the enhancement of the interlayer coupling strength and the geometrical overlap of phonon modes is not increased by modulating the LJ parameters in the simulations.

Fig. 4 – Phonon DOS of a graphene/h-BN bilayer system at 300 K for different interlayer coupling strength (a) $\mu=0.5$, (b) $\mu=1.0$, and (c) $\mu=2.0$. The overlapped areas are denoted by purple.

Thermal rectification is a phenomenon in which heat transport is preferred in one direction over the opposite and it can't be observed in the 2D system because the heat flux direction has no effect on the ITR of the system. It is attributed to the absolute lattice matching and highly symmetric atomic structure of the 2D system and good phonon matching between graphene and h-BN. It has been reported that the phonon spectra of h-BN and graphene are similar on the whole, implying that the thermal properties between these two materials are comparable [45]. Therefore, no thermal rectification is observed at the interface of the 2D system.

Fig. 5 - (a) ITR and (b) thermal rectification factor of a DWNT composed of a coaxial (6, 0) CNT inside a (15, 0) BNNT; (c) ITR and (d) thermal rectification factor of a DWNT composed of a coaxial (6, 0) BNNT inside a (15, 0) CNT, at different temperatures and LJ parameters

The ITR of 1D CNT/BNNT composite (Fig. 5(a) and (c)) is in an order of magnitude of 10^{-7} - $10^{-6} \text{ Km}^2/\text{W}$ and thermal rectification is observed in both of the DWNTs. The thermal rectification factor η , as shown in Fig. 5(b) and (d), is defined as

$$\eta = \frac{R_{i-o} - R_{o-i}}{R_{o-i}} \times 100\% \quad (7)$$

where R_{i-o} is the ITR as heat transfers from the inner nanotube to the outer nanotube and R_{o-i} is the ITR in the opposite direction. The positive value of η in both of the DWNTs means that heat energy prefers to transfer from the outer nanotube to the inner nanotube over the opposite direction no matter CNT acts as the inner or the outer tube of the CNT/BNNT hybrid system. The thermal rectification factor is affected by both temperature and coupling strength and its largest value could reach

about 90% in the case of this work. However, the influences of temperature and coupling strength on the thermal rectification factor of the two CNT/BNNT composites are quite different. For example, for Fig. 5(b) the maximum thermal rectification factor occurs at 500 K for different coupling strength while it's not the case for Fig. 5(d). The averaged thermal rectification factor at different temperatures increases with stronger intertube coupling strength for Fig. 5(d) while the thermal rectification factor with $\mu = 0.5$ is larger than that with $\mu = 1$ for Fig. 5 (b). Fig. 10 of [46] gives the ITR between Ar1 and Ar10 in different heat flux directions from 10 K to 80 K, the ITR decreases on average by about 15% when the heat flux direction is changed from Ar10 $\rightarrow$ Ar1 to Ar1 $\rightarrow$ Ar10, but the temperature dependence of the thermal rectification factor is not presented. By calculating a two-segment chain with the Frenkel-Kontorova (FK) model, Li et al. [47] observed the ratio of the positive and negative heat fluxes with the same temperature difference could be as large as 100 times for a weak interface coupling and the rectification could disappear with a strong interface coupling. In the case of this work, the validity of the ITR of the CNT/BNNT system can be guaranteed, however, the effects of temperature and coupling strength on the thermal rectification factor are still not very clear. Since the measurement is quite difficult to realize in the real experiments, more efforts on the thermal rectification effect of the 1D composite are need by various numerical simulations.

The phenomenon of thermal rectification in a CNT/BNNT system is similar with that in a double-walled CNT which is explained by the contraction principle. When a CNT is heated, it expands in the radial direction, and when it is cooled it contracts. In a double-walled CNT, when heat transfers from the outer to the inner CNT, the inner CNT expands on heating, while the outer CNT contracts upon cooling, improving mechanical coupling between the two CNTs. On the other hand, when heat transfers from the inner to the outer CNT, the mechanical expansion/contraction leads to less mechanical coupling as the heat-transfer process progress [35]. Furthermore, from the phonon DOS in Fig. 6, it is found that both of the graphs have a strong peak at around 48 THz for the outer nanotube and 46 THz for the inner nanotube, and the outer nanotube has more high-frequency phonons than the inner nanotube, which means

phonons of the outer nanotube could carry more energies to participate in heat transport across the interface than the inner nanotube and thus heat flows more easily from the outer towards the inner nanotube than the opposite direction. The thermal rectification in the 1D system is due to the atomic structural asymmetry between the outer nanotube and the inner nanotube. The phonon spectrum of CNT and BNNT in the 1D system is mismatched compared to that of graphene and h-BN in the 2D system.

Fig. 6 – Phonon DOS of (a) a coaxial (6, 0) CNT inside a (15, 0) BNNT and (b) a coaxial (6, 0) BNNT inside a (15, 0) CNT at a temperature of 300 K with intertube coupling strength $\mu = 1$. The overlapped areas are denoted by orange.

4. Conclusion

To summarize, MD simulations are employed using the LAMMPS package to study the heat performance at the interfaces of both 2D and 1D C/h-BN vdW heterostructures. The ITR of 2D graphene/h-BN bilayer system and 1D concentric CNT/BNNT hybrid system are estimated, within the lumped capacity method. The calculated ITR has an order of magnitude of 10^{-7} - 10^{-6} Km^2/W , and it decreases monotonically with temperature and coupling strength, consisting well with the

available results of the 2D system. At a high temperature, more high-frequency phonons are populated and thus available to be scattered, which enhances the thermal transport across the interface. By modulating the parameter in the LJ potential, the ITR is reduced through the enhancement of the coupling strength instead of the geometrical overlap of the phonon modes. Radial thermal rectification in the CNT/BNNT hybrid system is first proposed in this work, with a largest thermal rectification factor of $\sim 90\%$ and it is attributed to the mismatched phonon spectrum of CNT and BNNT in the 1D system compared to that of graphene and h-BN in the 2D system. The outer nanotube has more high-frequency phonons than the inner nanotube no matter the outer nanotube is CNT or BNNT in the CNT/BNNT hybrid system, which means phonons of the outer nanotube could carry more energies to participate in heat transport across the interface than the inner nanotube and thus heat prefers to transport from the outer nanotube towards the inner nanotube over the opposite direction. Results in this work help understand the heat transport properties of the newly emerging graphene based low-dimensional nanoheterostructures and they might be useful for opening up new opportunities for applications in phonon engineering and nanoelectronics.

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