



Molecular dynamics simulation of thermal boundary conductance between horizontally aligned carbon nanotube and graphene



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ABSTRACT

Molecular dynamics simulations are employed to investigate the thermal boundary conductance between a horizontally aligned carbon nanotube (CNT) and graphene. The results show that the thermal boundary conductance increases monotonically with the temperature and the interfacial van der Waals interaction strength. It is also found that the thermal boundary conductance demonstrates strong positive correlation not only with the CNT diameter but also with the system length until it reaches an elevated plateau. After incorporating organic molecules into the interface, the thermal boundary conductance is about one order of magnitude higher than that without organic molecules due to the enhanced matching level of phonon density of states. When tensile strain is applied along the transversal direction, the thermal boundary conductance decreases with increasing stretching strain without organic molecules, and the reduction can be prevented with additional organic molecules. Further analysis indicates that larger overlap between the phonon spectra of organic molecules and sp^3 hybridized C atoms can compensate for the softening of high-frequency phonon modes of sp^2 hybridized C atoms in graphene induced by tensile strain. This work provides guidance about tuning the thermal transport of C-based nanomaterials for applications in nanoelectronic devices.

1. Introduction

With the development of miniaturization, modern electronic devices are becoming faster and smaller in pursuit of better performance and portability. As the shrinking of feature size and the increase in operating frequency, more power is inevitably generated and must be taken away as quickly as possible. Heat dissipation and thermal management have become a great challenge in nanoscale thermal transport. Conventional semiconductor such as silicon is not adequate to extract waste energy fast enough. Hence scientists have to search for new alternative materials for efficient heat dissipation.

Recently, carbon nanomaterials, especially carbon nanotubes (CNTs) and graphene, have attracted extensive attention due to their excellent electrical and thermal properties. These two materials have revealed extremely high thermal conductivity along tube axial and graphene in-plane direction, respectively. Several review articles have made a comprehensive overview of thermal conduction researches on carbon nanotube and graphene. Despite significant variations in the reported experimental values of the thermal conductivity of carbon nanotube and graphene, a thermal conductivity as high as several thousands of watt per meter Kelvin is reached [1–3]. Superior but anisotropic thermal conductivity makes them the best heat conductor and

good candidates for nanoscale thermal management. However, when integrating these two materials into nanoelectronics, the thermal boundary resistance dominates the thermal transport across nanoscale interfaces instead of the high intrinsic thermal conductivity. For instance, the thermal conductivity of polymer composites by adding 1% volume fraction of CNTs is only ~ 0.4 W/mK, two times larger than that of pure polymers [4]. This less pronounced increase in thermal conductivity is attributed to the poor thermal coupling of the CNTs/graphene with the surrounding polymer matrix [5,6].

As an example of hybrid materials including graphene and CNTs, the pillared-graphene architecture by incorporating CNTs as interconnects between graphene nanoribbons (GNR) is appealing for thermal management applications. It is expected that there is a low thermal barrier for phonons flowing in such a novel architecture and thermal boundary resistance is maintained at a relatively low level. Because both materials are built from the same element carbon and arranged in a honeycomb lattice, the mismatch of phonon spectra is reduced, and thus enhances the thermal coupling between CNTs and graphene. Dimitrakakis et al. [7] reported the capability of hydrogen storage in pillared-graphene. Varshney et al. [8] investigated the thermal transport in a pillared-graphene network and found that the minimum interpillar distance and pillar length are key factors for

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Nomenclature

C_{CNT}	heat capacity of carbon nanotube
E	overlapped phonon energy of vibrational density of states
G	thermal boundary conductance
H	Planck constant
k_B	Boltzmann constant

L	system length
ΔT	temperature difference
T	relaxation time
X	scaling factor
N	frequency
γ	velocity

tailoring the thermal conductivity. Loh et al. [9] studied the effects of mechanical strain on the interfacial thermal resistance of the pillared-graphene architecture via molecular dynamics (MD) simulations. Their results showed that the interfacial thermal resistance could be tuned through mechanical strain by altering the interfacial phonon dynamics.

Apart from three-dimensional pillared-graphene nanostructure, a two-dimensional hybrid structure by integrating CNTs with monolayer graphene, called rebar graphene, has been proposed [10–12]. The horizontal CNTs serve as reinforcing bar for good mechanical flexibility. This planar CNT/graphene hybrid sheets are synthesized by simply annealing functionalized CNTs on Cu foils. Because of improved mechanical strength, rebar graphene can be free-standing on water and transferred onto substrates without a polymer coating [11]. Furthermore, unique optical and electrical properties are inherited from both graphene and CNTs. These intriguing features indicate that rebar graphene has potential applications as transparent conducting electrodes [11], metal-free electrocatalyst [13] and high-efficiency osmosis membrane [14].

Previous studies have been conducted on the interfacial thermal transport of bilayer heterostructures, such as graphene/silicene [15] and graphene/hexagonal BN [16]. However, in contrast to the comprehensive understanding of bilayer heterostructures, the thermal transport mechanisms across the interface between horizontal CNTs and the graphene have not been well studied.

In this paper, classical molecular dynamics simulation method is used to investigate the thermal boundary conductance between a horizontal CNT and graphene nanoribbons (GNR). The effects of temperature and interfacial interaction strength, diameter and length on the thermal boundary conductance are studied. Furthermore, we also investigate the dependence of thermal boundary conductance on molecular linkers and tensile strain in detail. Phonon spectra analysis is adopted to explain our findings.

2. Model and simulation setup

The atomic configuration of CNT/GNR interface is depicted in Fig. 1. A 5 nm long (10,10) single-walled CNT is horizontally aligned on the surface of the GNR. Different from the CNT/CNT interface, where point-contacts could be formed at the intersection points if CNTs do not align well. However, this problem does not exist at the interface of CNT/GNR, the horizontal CNT and GNR always form line-contacts. In our model system, the zigzag edge of the GNR is oriented along the tube axial direction. This indicates that C atoms in CNT and GNR share the same coordinate in longitudinal direction. The minimum distance between the CNT and GNR is set to be 0.34 nm and the width of the GNR is fixed at 4 nm. With regard to the effect of covalent binding, methylene (CH_2) is chosen as molecular linker to bridge the interface, as shown in the right panel of Fig. 1. The closest pair of C atoms across the interface is connected to molecular linkers. Periodic boundary condition is applied to the transverse and longitudinal directions, and free boundary condition is applied to the cross-plane direction.

All MD simulations are conducted using LAMMPS [17] package. The optimized Tersoff potential is used to describe the sp^2 C-C bonding interactions because of its accurate description of the anharmonicity and acoustic phonon dispersions [18]. The cross-plane van der Waals interactions between CNT and GNR are modeled with the 12-6 Lennard-

Jones (LJ) potential, written as

$$V(r) = 4\chi\epsilon[(\sigma/r)^{12} - (\sigma/r)^6] \quad (1)$$

where ϵ is the well-depth energy, σ is the equilibrium distance and r is the interatomic distance. The χ is an adjustable parameter to control the interfacial interaction strength. These parameters are described by a united atom model with detailed geometrical and force field parameters taken from Ref. [20]. The bond length and bond angle between C atoms in CNT or GNR and methylene molecular linkers are 0.153 nm and 114° , respectively.

A nonequilibrium MD simulation method is implemented to calculate the thermal boundary conductance. At first, we carry out an energy minimization to fully optimize the structure by conjugate gradient method. Then, we relax the system at the desired temperature T with NVT (constant volume and temperature) ensemble for 100 ps with a time step of 0.5 fs, using Nosé-Hoover thermostat [21,22]. Following NVT relaxation, the system is switched to the NVE (constant volume and energy) ensemble for another 100 ps to ensure that the total energy is conserved. As the equilibrium state is reached, a temperature difference ΔT is applied by instantaneously heating the CNT to $T + \Delta T$, while maintaining the GNR at T for 50 ps. Afterward, the system continues to relax with NVE ensemble to mimic the heat transfer process. We then record the temperature difference between the CNT and GNR as a function of time. Without additional coupling to an external thermostat, the temperature difference ΔT decays in an exponential manner with a single relaxation time τ as

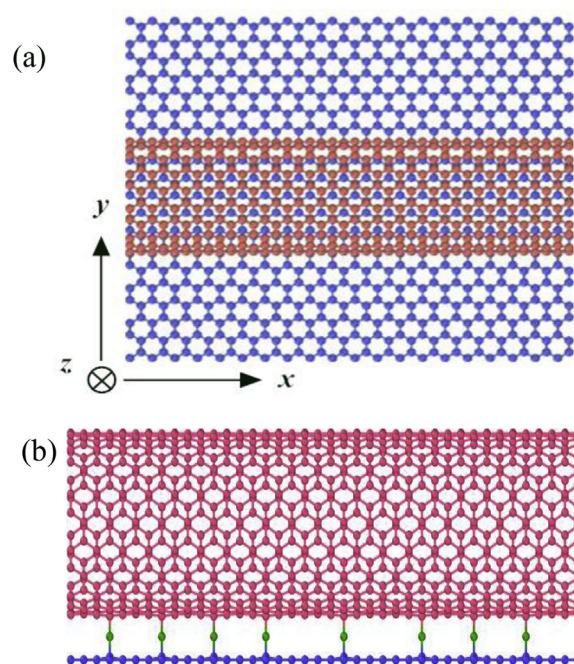


Fig. 1. (a) The schematic model of a 5 nm long (10,10) single-walled CNT horizontally aligned on the surface of GNR. (b) Side view of horizontal CNT/GNR interface with the united atom CH_2 molecular linkers. The molecular linkers are distributed regularly along the longitudinal direction.

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