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Dependence of carbon nanotube array-silicon interface thermal conductance on array arrangement and filling fraction

Ya Feng, Jie Zhu*, Dawei Tang

Key Laboratory of Ocean Energy Utilization and Energy Conservation of Ministry of Education, Dalian University of Technology, Dalian, Liaoning 116024, China

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ABSTRACT

Carbon nanotube (CNT) is a promising candidate of thermal interface material for micro/nano-scale devices due to its ultra-high axial thermal conductivity. However, low interface thermal conductance between CNT and other materials restricts its effectiveness in the thermal management. We use non-equilibrium molecular dynamics (NEMD) method to investigate the factors that possibly influence the interface thermal conductance between vertical CNT array and silicon substrate. The dependence of the interface thermal conductance on the arrangement of CNT (aligned and crossed), filling fraction (0.14–0.70), CNT diameter (6.88–35.75 Å), temperature (200–400 K), and van der Waals force among the CNTs are studied in detail. From the simulation results, the enhancement of the interface thermal conductance difference caused by CNT-array filling fraction in this work reaches to 91%, and that value caused by the arrangement of CNT on silicon is as high as 84%. The mechanism of heat transport across the interface between CNT array and silicon substrate is discussed by comparing the vibrational densities of states (VDOS) of atoms from both sides under different conditions.

1. Introduction

With its high elastic modulus [1] and axial thermal conductivity [2,3], CNT is a promising candidate of thermal interface material (TIM) for micro/nano-scale devices to enhance the heat dissipation which is vital for the safety and steady of devices operation. Experiments [4–8] and simulations [9–13] have been widely conducted to investigate the thermal behaviors of CNTs under different surrounding conditions, and the results suggest that low interfacial thermal conductance [14,15] bottles the heat transport through CNT-TIM, despite the high intrinsic thermal conductivity of CNTs. Compared with the covalently bonded interface (growth side), the poor adhesion on the growth-opposite side of CNT array leads to even more serious thermal interface resistance due to weak van der Waals interactions [16–18]. Most of the experimental reports on the interfacial thermal conductance are performed with CNT arrays other than single CNT for seeking much easier experiment operations and sample preparations [19–22], while previous simulation studies are constructed with single CNT on substrate [23–25]. Moreover, few simulation works have concerned the interfacial thermal conductance of CNT array as TIM across the growth-opposite side, which will be the prior consideration in the present work.

In this work, our purpose is to reveal how and how much we can enhance the interfacial thermal conductance across the growth-opposite side between CNT array and silicon, using non-equilibrium molecular dynamics (NEMD) method [18,26,27]. The dependence of the interfacial thermal conductance on CNT array filling fraction (the ratio of CNT sectional area to surface area of silicon thin layer), the arrangement of CNT, CNT diameter, temperature, and van der Waals force among tubes are investigated. Moreover, the VDOSs of interfacial atoms are analyzed to further understand the mechanism of interfacial heat transport between CNT array and silicon thin layer under different conditions. The present work indicates that the aligned arrangement of CNT on Si substrate is more advantageous to interfacial thermal conductance in some diameter range, which would provide fresh ideas to the manipulation of interfacial thermal conductance through patterned CNT growth.

2. Modeling and simulation method

The CNTs investigated in this work are all single-walled (SWNT). The CNT-array/silicon simulation structure is demonstrated in Fig. 1. There is no bend or buckle of CNTs at the interface because the length of CNTs in our simulation is only 2.5 nm. This is the major reason that we do not investigate the longer CNT systems, and the CNT size effects on the interface thermal transport between single CNT and substrates can be found in our previous report [25]. There are two kinds of arrangements of CNT array on silicon thin layer to be simulated here, one is aligned arrangement as shown in Fig. 1(a), and the other is crossed

* Corresponding author.
E-mail address: zhujie@dlut.edu.cn (J. Zhu).

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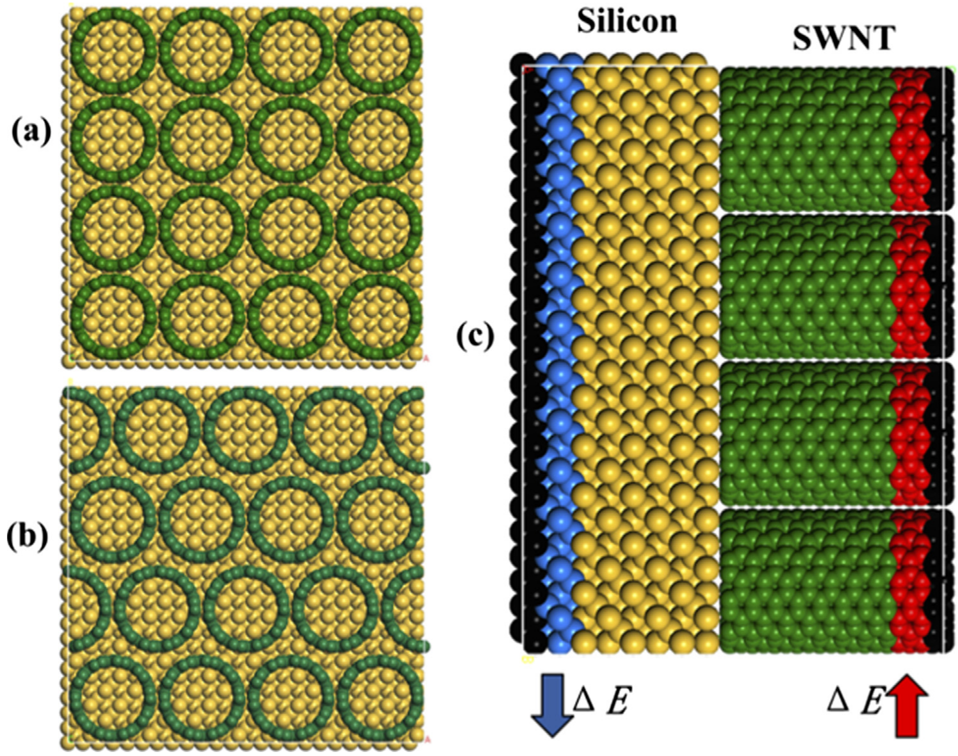

Fig. 1. CNT array-Silicon simulation structure: (a) top view of aligned arrangement of CNT; (b) top view of crossed arrangement of CNT; (c) the growth-opposite interface, heat flux is added in the red region (heat source) in CNT array and subtracted from the blue region (heat sink) of Silicon thin layer with the same amount.

arrangement shown in Fig. 1(b).

In simulations, periodic boundary condition is applied in x and y directions, but free boundary condition in z direction (CNT axial orientation). The number of CNT in each simulation unit keeps the same for all the simulations in this study. Therefore, to guarantee that the radial distance between two tubes belonging to two adjacent simulation units keeping the same with that in one simulation unit, the size of silicon substrate in x and y directions has to be adjusted with the different diameters of CNTs. Therefore, we build three simulation groups, whose names are S, M, and L respectively. The structural parameters of these three groups are specified in Table 1, with the silicon sizes indicated. Every group includes several structures which successively increases CNT diameter. Moreover, every simulation structure is carried out with two CNT arrangements. Therefore, within every group, we can discuss the relationship of interfacial thermal conductance with filling fraction, CNT diameter and compare the effect of CNT arrangement.

The adaptive intermolecular reactive empirical bond order (AIREBO) potential [28] is used to model the interactions between carbon atoms (C-C) in CNTs. The long-range interactions between C atoms of different tubes are modeled by the similar standard Lennard-Jones (LJ) potential in AIREBO, whose cutoff is 10.2 Å. That indicates there are two set simulations (CNT-array (12, 12) in group M and CNT-array (20, 20) in group L, see Table 1) in our work are out of this long LJ tube-tube interactions. Moreover, Tersoff potential [29,30] is

Table 1
Details of every different structure studied in our simulations.

Group name	CNT chirality	CNT diameter (Å)	CNT distance (Å)	Filling fraction	Other information
	(5,5)	6.88	9.4121	0.27637	Si substrate: 6 × 6 × 4 supercell
	(6,6)	8.25	8.0421	0.3314	
S	(7,7)	9.63	6.6621	0.38683	x × y × z = 32.5842 Å × 32.5842 Å × 21.7228 Å
	(8,8)	11.00	5.2921	0.44186	
	(9,9)	12.38	3.9121	0.4973	
	(10,10)	13.75	2.5421	0.55233	CNT: 10 units; 24.94 Å long
	(12,12)	16.50	10.6535	0.24022	Si substrate: 10 × 10 × 4supercell
	(13,13)	17.88	9.2735	0.26031	
	(14,14)	19.25	7.9035	0.28026	x × y × z = 54.3070 Å × 54.3070 Å × 21.7228 Å
M	(15,15)	20.63	6.5235	0.30035	
	(16,16)	22.00	5.1535	0.32029	
	(17,17)	23.38	3.7735	0.34038	CNT:10units; 24.94 Å long
	(18,18)	24.75	2.4035	0.36033	
	(20,20)	27.50	10.5149	0.2045	Si substrate: 14 × 14 × 4 supercell
	(21,21)	28.88	9.1349	0.21476	
	(22,22)	30.25	7.7649	0.22494	x × y × z = 76.0298 Å × 76.0298 Å × 21.7228 Å
L	(23,23)	31.63	6.3849	0.23521	
	(24,24)	33.00	5.0149	0.24539	
	(25,25)	34.38	3.6349	0.25566	CNT: 10 units; 24.94 Å long
	(26,26)	35.75	2.2649	0.26584	