Supporting Information

Heat Conduction in Double-walled Carbon Nanotubes with Intertube Additional Carbon Atoms

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I. MD simulation details

In MD simulations, the periodic boundary condition was applied along the tube axis. A time step of 0.50 fs was imposed. The interactions between carbon atoms of DWCNTs with added atoms were based on the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential [1]

$$E = \frac{1}{2}\sum_{i}\sum_{j\neq i}\left[E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k\neq i,j}\sum_{l\neq i,j,k} E_{kijl}^{TORSION}\right] \tag{1}$$

where E_{ij}^{REBO} is the REBO potential function, E_{ij}^{LJ} adds longer-ranged interactions, $E_{kijl}^{TORSION}$ is an explicit 4-body potential which represents dihedral angle preferences. It should be pointed out that the term of $E_{kijl}^{TORSION}$ has been ignored in this work.

The DWCNT with added atoms was axially partitioned into 50 slabs for temperature recording and control. Firstly, the DWCNT with added atoms was heated and kept at 300 K for 300 ps in the Nosè-Hoover thermostat to reach a thermal equilibration. After that, two slabs which are separated at half of the nanotube length were chosen as hot and cold domains, as illustrated in Fig. 1. A heat flux then transferred between these two slabs through exchanging momentum between the 'hottest' atom in cold slab and the 'coldest' atom in the hot slab. The momentum exchanging was performed every 10 fs. This process was equilibrated under a constant-energy micro-canonical (NVE) ensemble for 400 ps. The heat flux J was computed as

$$J = \frac{\sum_{N_{transfer}} \frac{1}{2}(mv_h^2 - mv_c^2)}{2At} \tag{2}$$

where $N_{transfer}$ is the number of momentum exchanges that have been performed, A is the cross-section area, t is the summation time, v_h and v_c are the velocities of the 'hottest' atom in cold slab and the 'coldest' atom in the hot slab, respectively.

The temperature profile was averaged over a 50 ps time interval. Finally, the thermal conductivity can be calculated according to the Fourier's law

$$\kappa = \frac{J}{\partial T / \partial x} \tag{3}$$

In this paper, we treated the cross-sectional area A of DWCNTs as the total area of inner and outer annular rings. Therefore, A was calculated as

$$A = 2\pi\delta(R_i + R_o) \tag{4}$$

where δ=0.34 nm is the wall thickness of the nanotube. R_i and R_o are the radii of the inner and outer tube walls, respectively.

II. Orthogonal array testing strategy

Orthogonal array testing strategy is a black box testing technique that is a systematic, statistical way of software testing. It is used when the number of inputs to the system is relatively small, but too large to allow for exhaustive testing of every possible input to the systems [2]. In this paper, three structural factors made comparisons in this paper are the tube length (L), the density of chosen cross-sections to add atoms (ρ_1), i.e. the number of cross-sections per nanometer along the tube length, and the number of added atoms at each cross-section (ρ_2), respectively. The cross-sections were uniformly arranged along the tube length direction and the added atoms at each cross-section were set symmetrically. Factors and levels for orthogonal array testing strategy are listed in Table 1. In this study, totally 16 examples are carried out and the results under the temperature of 300 K are presented in Table 2. The largest reduction in thermal conductivity is up to 54%. Table 3 shows the computed average index *Ki* (the average value of the results in the level *i*) and extreme difference *R* (the difference between maximum and minimum values of average index *Ki*).

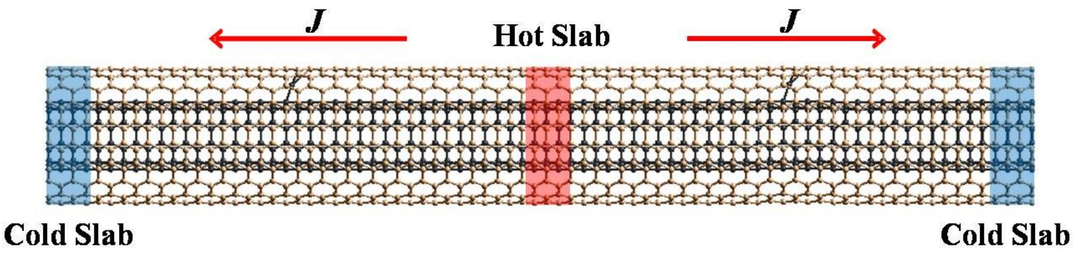

Figure. 1 Settings of the hot and cold slabs in the model (heat flux *J* is transferred from the hot to cold slab)

Table 1. Factors and levels for orthogonal array testing strategy

variable	level *i*			
	1	2	3	4
L, length(nm)	5	10	15	20
ρ_1, denisty of cross-sections to add atoms	0.4	0.6	0.8	1.0
ρ_2, number of added atoms at each cross-section	1	2	3	4

Table 2. Results of thermal conductivity

No.	*L*, length(nm)	ρ_1, denisty of cross-sections to add atoms	ρ_2, number of added atoms at each cross-section	*k*, thermal conductivity（W/(m·K)）		reduction in thermal conductivity (%)
				DWCNT with intertube carbon atoms	empty DWCNT	
1	5	0.4	1	13.1	16.3	19.6
2	5	0.6	2	11.6	16.3	28.8
3	5	0.8	3	7.5	16.3	54.0
4	5	1	4	9.0	16.3	44.8
5	10	0.4	2	18.2	24.8	26.6
6	10	0.6	3	14.5	24.8	41.5
7	10	0.8	4	12.1	24.8	51.2
8	10	1	1	21.0	24.8	15.3
9	15	0.4	3	22.2	37.5	40.8
10	15	0.6	4	22.7	37.5	39.5
11	15	0.8	1	29.5	37.5	21.3
12	15	1	2	26.4	37.5	29.6
13	20	0.4	4	25.8	48.5	46.8
14	20	0.6	1	39.6	48.5	18.4
15	20	0.8	2	27.7	48.5	42.9
16	20	1	3	27.7	48.5	42.9

Table 3. Results of extreme difference *R*

	L, length(nm)	ρ_1, density of cross-sections to add atoms	ρ_2, number of added atoms at each cross-section
K1	36.8	33.5	18.7
K2	33.7	32.1	32.0
K3	32.8	42.4	44.8
K4	37.8	33.2	45.6
R	5.0	8.9	26.9

Ki is the average value of the results in the level *i*;

R is the difference between maximum and minimum values of average index *Ki*

References

1. Stuart S J, Tutein A B and Harrison J A 2000 The Journal of Chemical Physics 112:6472.
2. Roger S P. Software Engineering: A Practitioner's Approach (6th ed.). Boston: McGraw-Hill; 2005.