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THE EFFECT OF THERMAL INTERFACIAL RESISTANCE ON CARBON NANOTUBE AND ETHYLENE GLYCOL BASED NANO-FLUID: A MOLECULAR DYNAMICS APPROACH

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ABSTRACT

It is founded that carbon nanotube CNT has the property to boost the heat transfer rate at liquid-solid interface although it has some drawbacks due to the resistance of thermal interfacial. The thermal inter-facial resistance occur due to the mismatch of vibrational at interface, which place a key duty in energy transfer at the boundaries. Some little output has documented on the impact of carbon nano-tube diameter effect on the resistance by the vibrational-mismatch study. Molecular dynamics (MD) is used to enquire the effect of SWAC (single walled armed chair) on diameter of CNT, on interfacial thermal resistance between ethylene glycol and carbon nano-tube. This study is attempt to know the phenomenon of heat transfer at the interface of arm chair CNT and ethylene glycol, by examine the spectra of vibrational of CNT and ethylene glycol, vibrational mismatch at the contact is quantified. For the bigger diameter nano-tubes a substantially higher thermal interfacial resistance is reported. This is cause to high vibrational mismatch existing at large diameters. Due to the lower overlap-region between the vibrational-density states of CNT and ethylene glycol molecules which results in a bigger vibrational mismatch for larger diameters CNT. The importance of smaller diameter CNT is cooling application s is highlighted by the low thermal interfacial resistance that's all diameter CNT exhibit. This low resistance allows for effective heat transfer at the interface

INTRODUCTION

The carbon nanotube CNT is discover in 1991 it made a revolutionary change in science and technology research field. Because CNT has a good thermal conductivity (noted to be high as 6500 W/m-k, equally to 18 times of bulk metallic copper), these materials has the most important is transfer applications. In this experiment, molecular dynamics simulation has performed to know the reaction of CNT diameter on the interfacial thermal resistance between ethylene glycol and CNT. the simulation process is bounded to SWAC CNT. The aim of this study is, using vibrational overlapping

spectrum between ethylene glycol and CNT figure out the phenomenon of heat transfer at interface more accurately. The individualistic simulations are performed in molecular dynamics (MD) on SWAC CNT having chirality as (25,25),(20,20),(15,15),(10,10) and (5,5) neighboring by ethylene glycol molecules using software named as LAMMPS the CNT diameter is based on its chirality, it calculate as per the formula given in literature. This study has divided into parts containing of setup, procedure and simulations, followed by the obtained results with its discussion and conclusion at end

SIMULATION SETUP AND PROCEDURE

MD Simulations are good range of applications for calculating the molecular level reactions and thermos-chemical properties and etc. Algorithm of varlet is used to measure the velocity and positions of the atoms at a point of time step by applying integration on newton's motion of Equation. The potential energy function is depended on the position of atoms, which are presented in the simulation. The non bonded and bonded energy interactions given as follows,

$$V(r) = V_B(r)+V_{N-B}(r) \quad (1)$$

The interactions between the bonds states that angle between the bonds, bonds torsional motions.Thenon-bonded interactions calculated by Van-der Walls equations.

$$V_{N-B}= V_{vdw}+V_{coul} \quad (2)$$

The Van-der Walls potentials is modified by Jones Lennard (JL) 6:12 potentials and defind as,

$$V_{vdm} = \sum_{i\neq j} 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] \quad (3)$$

Where ε and σ are LJ parameters. The electro-static energy interactions as noted by coulombic potential as,

$$V_{coul} = \sum_{i\neq j} 4\varepsilon_{ij}\frac{q_i q_j}{r_{ij}} \quad (4)$$

in this qj, qi are the charge on atom j and i of atom pair ij.the interaction between two atoms are given by the Berthelot-Lorentz mixing rules,

$$\sigma_{ij} = \frac{\sigma_{ii}+\sigma_{jj}}{2} \quad (5)$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_{ii} * \varepsilon_{jj}} \quad (6)$$

the domain of the MD simulation contains previously calculated ethylene molecules in a cube of dimensions 6 nm having the periodic boundary conditions depending on the CNT diameter. The scaling of velocity is carried out as follows

$$\frac{T_{req}}{T_{base}} = \left(\frac{V_{req}}{V_{base}}\right)^2 \quad (7)$$

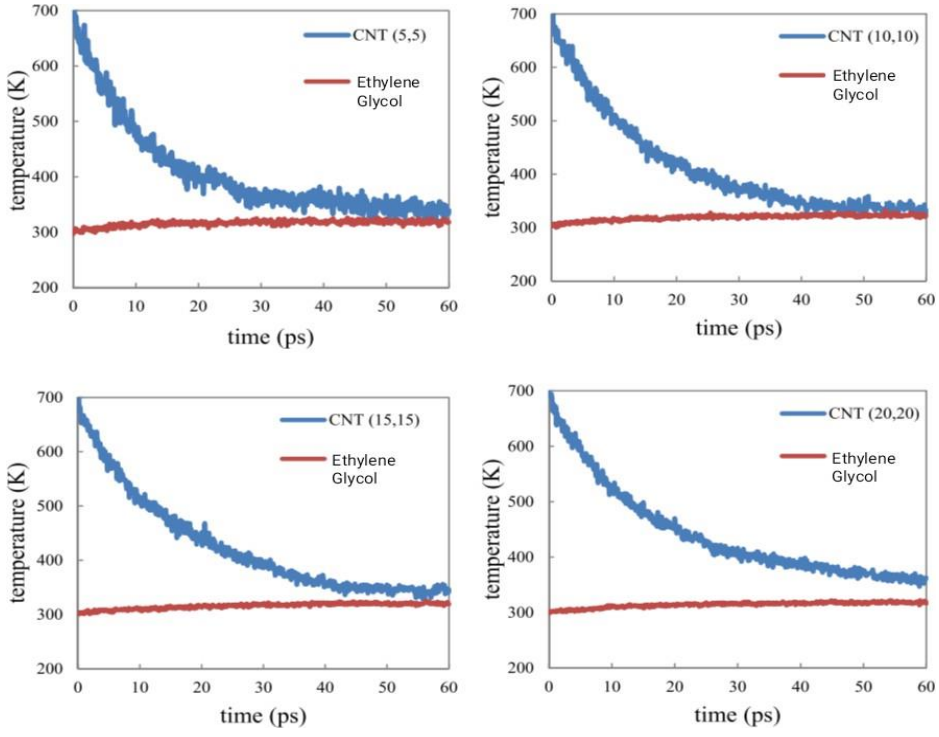
Where T_{req} and T_{base} are the temperatures of CNT required, V_{req} ,V_{base} are velocities of carbon atoms. Now the simulation run by the LAMMPS code, it helps to give the desire conditions to get the required outputs.

Table1. Parameters used in simulations

CNT (chirality)	diameter of Nano-tube (nm)	Carbon atoms (Nc)	$C_2H_6O_2$ molecules(N_{EG})	Ratio (N_{EG}/Nc)
(5,5)	0.679	500	1800	3.60
(10,10)	1.356	1000	3600	3.60
(15,15)	2.034	1500	5400	3.60
(20,20)	2.713	2000	7200	3.60
(25,25)	3.391	2500	9000	3.60

RESULTS AND DISCUSSION

Fig.1 generated by using molecular dynamic simulations of SWCNT placed at center neighboring by ethylene glycol molecules. The temperature decay of CNT temperature, during the relaxation-period plotted in different diameters of nano-tube it shows that the temperature of CNT falls faster and gives heat to the ethylene glycol molecules, the temperature raise in all simulations are approximately same, it shows that the interfacial thermal resistance is same for all the simulations. The logarithmic-decay of the temperature between the ethylene glycol and nano-tube for all the cases. As shown in Fig.2 the temperature-decay of larger diameter CNT is slower than the smaller diameter CNT. The slope of inverse of this decay with respective time gives the time constant which helps to calculate the interfacial thermal resistance from that the time constant for CNT (25,25) is larger than the CNT (5,5). The interfacial thermal resistance calculated by formula (8)



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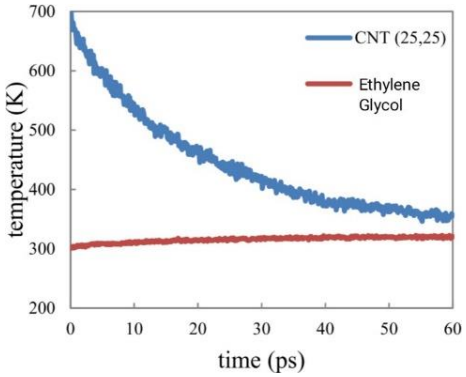

Fig. 1 Temporal variation of CNT temperature and ethylene glycol molecules in the production run (NVE ensemble).

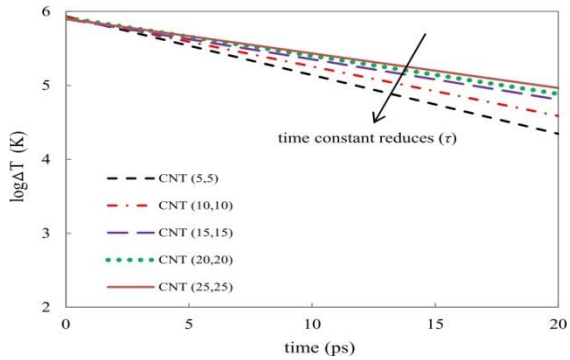

Fig. 2 Temporal variation of CNT temperature and ethylene glycol molecules in the production run (NVE ensemble).

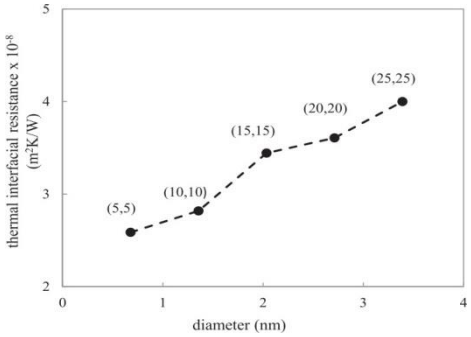

Fig. 3 Effect of nano-tube diameter on the interfacial thermal resistance.

As shown in Fig.2 the temperature-decay of larger diameter CNT is slower than the smaller diameter CNT. The slope of inverse of this decay with respective time gives the time constant which helps to calculate the interfacial thermal resistance from that the time constant for CNT (25,25) is larger than the CNT (5,5). The interfacial thermal resistance calculated by below formula

$$\tau = \frac{mc_T R_k}{A_{CNT}} \qquad (8)$$

Where τ the time constant, *m* is is the mass of the nano-tube $c_T$and A_{CNT} are the specific capacity and area of surface of the nano-tube respectively and R_k is the interfacial thermal resistance. The specific heat capacity of the nano tube depends on the diameter of CNT. The mass is calculated by the atoms are presented in the nano-tube. Table.2 tells the constant of time for various diameters of CNT. The time constant values are helps in finding the interfacial thermal resistance between ethylene glycol and CNT at the interface and calculate the diameter effect on CNT. The interfacial thermal resistance for CNT (5,5) obeys the value of N.Singh et al.[4].To study of overlapping of vibrational density, between the ethylene glycol and CNT vibrational spectrum analyzed. The less frequency modes are

take a major role in phenomenon of heat transfer at interfaces. Liquid molecules ae interact toughly with RBM and made mechanism for heat transfer.

Table.2 nano-tube diameter effects on time constant

CNT (chirality)	diameter of Nano-tube (nm)	Time constant (ps)
(5,5)	0.679	13.10
(10,10)	1.356	14.94
(15,15)	2.034	18.36
(20,20)	2.713	19.40
(25,25)	3.391	21.38

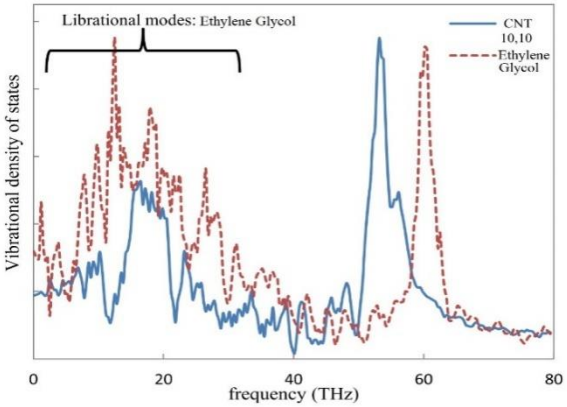

Fig.4 Carbon nano-tube vibrational density of states with ethylene glycol molecules just neighbouring the nano-tube

Fig.5 tells the overlapping region between ethylene glycol molecules and CNT with different diameters.

Table 3Summarized simulation results showing the effect of diameter of Nano-tube.

CNT (chirality)	diameter of nano-tube d (nm)	time constant t (ps)	thermal interfacial resistance R_k x 10-8 (m^2 K/W)	overlapping ratio
(5,5)	0.679	13.10	2.59	0.81
(10,10)	1.356	15.00	2.81	0.76

(15,15)	18.36	3.45	0.74	
(20,20)	19.40	3.60	0.72	
(25,25)	21.38	4.00	0.69	
overlapping ratio $=2 \times \frac{A_{over}}{A_{EG}+A_{CNT}}$				

The relation between the vibrational density and thermal resistance is when the vibrational density high the thermal resistance is low. The Table.3 tells the summirised results of simulations .by that CNT (5,5) has highest overlapping ratio.

Conclusions

The MD simulation are conducted to know the diameter effect on the carbon nano-tube of walled single by the interfacial thermal resistance between ethylene glycol molecules and CNT the analysis is conducted based on the ratio of overlapping as mentioned as earlier. The obtained resistance values during simulations on CNT (5, 5) is in best matching with the available literatures. When the simulations are conducted on larger diameters found that the thermal time constant of temperature-decay raises with the increment of nano-tube diameter it leads to the raise in resistance due to interfacial thermal Analysis of vibrational-spectrums of nano-tube and neighboring ethylene glycol to appraise the vibrational-mismatch explains need of the interfacial thermal resistance on the diameter of nano-tube. Results are prove that small diameter has less vibrational mismatch and larger diameters has more vibrational mismatch. The high vibrational-mismatch leads to poor connection between CNT atoms and ethylene glycol molecules it causes weak connection at interface. This finally decreases the interfacial heat transfer, in which increases the thermal interfacial resistance. This study is a small initial work to develop a good relationship between vibrational mismatch and thermal l resistance interfacial.To obtained high enhancement in transfer of heat, the Arm Chair CNT due to its higher over lapping ratio and lower interfacial thermal resistance, a small diameter should be preferred.

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