

## Thermal characteristics of defective carbon nanotube-polymer nanocomposites

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**Abstract.** The interfacial thermal resistance of pristine and defective carbon nanotubes (CNTs) embedded in low-density polyethylene matrix is studied in this paper. Interface thermal resistance in nanosystems is one of the most important factors that lead to the large variation in thermal conductivities in literature and the novelty of this paper lies in the estimation of the interfacial thermal resistance for defective nanotubes-systems. Thermal properties of CNT nanostructures are estimated using molecular dynamics (MD) simulations and the simulations were carried out for various temperatures by rescaling the velocities of carbon atoms in the nanotube. This paper also deals with the mesoscale thermal conductivities of composite systems, using effective medium theories by considering the size effect in the form of interfacial thermal resistance and also using the conventional micromechanical methods like Hashin-Shtrikman bounds and Wakashima-Tsukamoto estimates.

**Keywords:** carbon nanotube; molecular dynamics; universal force field potential; interfacial thermal resistance; stone-wales defect; effective medium theories; thermal conductivity.

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### 1. Introduction

Theoretical models and experimental studies have predicted that an addition of even a low volume fraction of CNTs would result in an increase in thermal conductivity of a composite system (Bryning *et al.* 2005, Gao *et al.* 2007, Strauss and Pober 2006). CNTs as potential composite reinforcements have many advantages over conventional fibers and enhanced thermal and

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mechanical properties of CNT are some of the primary reasons. CNT based composites are analyzed by considering the CNT as dispersed in a matrix and the interactions of the atoms of the CNT with the atoms of the matrix molecules is being studied by MD simulations (Griebel and Hamaekers 2004). The analysis of the problem is different from a conventional fiber composite material in the sense that the fiber phase interacts with the matrix phase through molecular interactions. In a conventional composite material analysis, the material/mechanical properties of the participating phases are widely studied and accepted. This is however not the case with the nanometric sized fibers, as the material properties are still being debated and even weak molecular interactions is found to alter the overall properties drastically (Chandra *et al.* 2004).

An important feature that is least understood in thermal analysis is the variation of the interfacial thermal properties of various types of nanocomposite systems, especially for the systems composed of nanotubes with defects. Recently, Unnikrishnan *et al.* (2008) predicted a significant effect on the interfacial thermal resistance of nanotubes when immersed in water, however no such works exists on the interfacial thermal characteristics of carbon nanotubes with defects.

The most common method of estimating the thermal properties of CNT nano-composites is through the estimation of thermal conductivities of the fiber material (Li and Wang 2005, Yokota *et al.* 2003). However it has been established by various studies that their mesoscale thermal conductivities are vastly influenced by the interfacial characteristics (Unnikrishnan *et al.* 2008, Xue *et al.* 2003, Xue 2006). Interface thermal resistance in nanocomposites or nanosystems is one of the most important factors that contributed to the large variation in the reported values of thermal conductivities in literature. For applications of nanocomposites stiffeners and as thermal conductors or insulators, use of longer nanotubes would be beneficial. However, as the length of the nanotube increases the number of bonding abnormalities like Stone-Wales defects also increases. There have been numerous studies on the quantum, electronic characteristics (Dinadayalane and Leszczynski 2007, Tserpes and Papanikos 2007, Vandescuren *et al.* 2007, Yoshiyuki *et al.* 2004) and mechanical characterization of Stone-Wales defects (Belytschko *et al.* 2002, Troya *et al.* 2003, Tserpes and Papanikos 2007).

The effect of defects on the thermal properties of nanotubes as well as the thermal properties of nanocomposite systems with defective nanotubes has not been reported in the literature. The motivation of this study is to perform detailed analyses of the thermal characteristics of polymer structures reinforced with defective nanotubes and compare the properties with polymer structures reinforced with defect-free nanotubes. One of the significant contributions of this paper is the estimation of the effect of the so-called Stone-Wales defect (to be discussed in the sequel) on the interfacial thermal resistance of the single walled nanotubes and the mesoscale effective thermal conductivities of polymeric nanocomposite systems. The thermal conductivities are estimated using the two effective medium theories that take into consideration the interfacial thermal effects and subsequently comparing with the lower and upper bounds from well known micromechanical methods. All molecular dynamics simulations in this study were performed using Cerius2 (version 4.6, Accelrys, Inc.) simulation package.

The paper is organized as follows. Section 2 describes the outline of the simulation procedure for the estimation of interfacial thermal resistance of pristine and defective carbon nanotube nanocomposite systems. Effective medium theories and homogenization bounds are described in Section 3 for nanocomposite systems, followed by a discussion of the results in Section 4, and the paper concludes with a summary in Section 5.

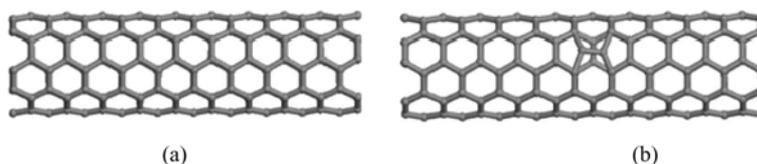


Fig. 1 (a) Defect free nanotube and (b) Nanotube with a Stone-Wales defect

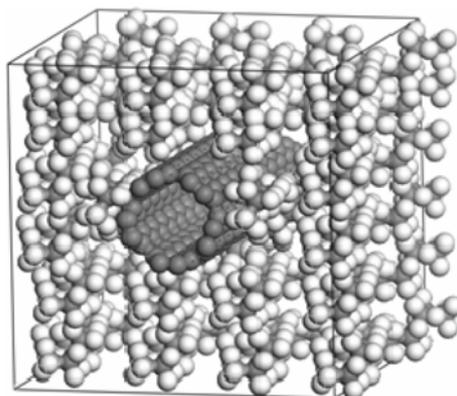


Fig. 2 Initial state of unit cell with single walled nanotube embedded in low density polyethylene matrix

## 2. Thermal analysis of defective carbon nanotube systems

One of the advantages of atomistic simulation is the ease with which various configurations can be studied when compared to an experimental investigation of CNT. Experimental investigations are extremely difficult as they are limited by the availability of high quality defect free CNTs of sufficient length (Fig. 1a) (Laborde-Lahoz *et al.* 2005). Perfect formation of nanotubes is always not possible to obtain and therefore the analysis of defects in nanotube is very essential. Stone-Wales defect is one of the significant abnormalities that can occur in a nanotube. A Stone-Wales defect is formed when a C-C bond in a hexagonal system is rotated  $90^\circ$  to form a pentagon-heptagon pair as shown in Fig. 1b. It has been estimated that Stone-Wales defects are normally observed in long nanotubes.

Molecular dynamics (MD) enables the computation of the trajectories of atoms by integrating Newton's second law of motion. It predicts the mechanical force field that exists in an atom due to interactions from the surrounding atoms by means of a potential field. The general-purpose Universal Force Field (UFF) of Cerius<sup>2</sup> (version 4.6, Accelrys, Inc.) is used in the present simulations. The universal force field is based on simple relations having parameters that depend on the type of element, hybridization and connectivities. The UFF includes hybridization dependant atomic bond radii, hybridization angles, van der Waals parameters, torsional and inversion barriers and effective nuclear charges. The potential energy of a molecule is the result of a series of superposition of various two-body, three and four body interactions (Rappe *et al.* 1992).

An armchair single-walled nanotube (5,5) with a diameter of  $7 \text{ \AA}$  and a double-walled nanotube having an inner (4,4) nanotube is used for the molecular dynamic simulations corresponding to a nanotube length of  $\sim 23.0 \text{ nm}$  with 200 atoms, and surrounded by polyethylene molecules (Fig. 2). The systems were equilibrated for 1 ps (1000 steps) and the temperature scaling was carried out in 8 ps as an NVT ensemble (8,000 steps). During the minimization and NVT processes, the atoms in

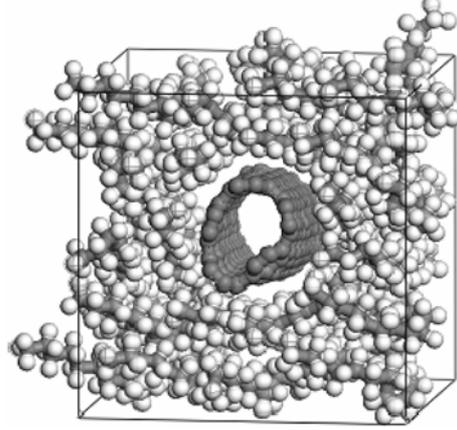


Fig. 3 Final state of unit cell of carbon nanotube in LDPE

the periodic unit cell are allowed to equilibrate within the fixed MD cell and periodic boundary conditions are applied in all directions. The nanotube ensembles were equilibrated and brought to the required temperature by similar set of thermostat algorithms and the final state of the unit cell is shown in Fig. 3. The simulated system and the heat bath couple to form a composite system. The conservation of the energy still holds in the composite system but the total energy of the simulated system fluctuates.

The nanotubes were equilibrated and brought to the base temperature (300 K), and subsequently the temperature of the central nanotube (nanotube in the composite unit cell) was raised to the predefined temperature. This rescaling was carried out by a rescaling of the velocities of the individual atoms of the nanotube instantaneously (Clancy and Gates 2006, Huxtable *et al.* 2003, Shenogin *et al.* 2004) as given in Eq. (1).

$$v_{new} = v_{old} \left( \sqrt{\frac{T_{target}}{T_{system}}} \right) \quad (1)$$

where  $T_{target}$  is the target temperature to scale to,  $T_{system}$  is the temperature of the system having velocities  $v_{old}$  and the final scaled velocity is  $v_{new}$  for each CNT atom in the ensemble. The modified ensemble is now allowed to relax under constant energy. The difference in temperature between the atoms of the CNT and the water molecules including the additives are now plotted against the MD time steps.

The interfacial thermal barrier resistance also known as the Kapitza resistance (Jiajun and Xiao-Su 2004) offers resistance to heat flow and reduces the effective conductivity of a fiber in a composite medium. The interfacial thermal resistance depends on the time constant  $\tau$  which is the slope of temperature decay of nanotube with the surrounding matrix and also depends on the nanotube heat capacity,  $C_T$  and the thermal resistance of the nanotube-matrix interface  $R_k$ .

$$\tau = R_k \left( \frac{1}{A_T / C_T} \right) \quad (2)$$

where  $A_T$  is the area of the nanotube and  $C_T / A_T$  is the heat capacity per unit area of the nanotube and is usually taken as  $5.6 \times 10^{-4} \text{ J/m}^2\text{K}$  (Clancy and Gates 2006, Huxtable *et al.* 2003, Shenogin *et al.* 2004) for carbon nanotubes.

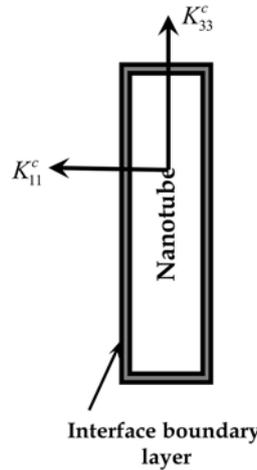


Fig. 4 Composite unit cell of a nanotube coated with a very thin interfacial thermal barrier layer

### 3. Mesoscale thermal analysis

Effective medium theories and mathematical homogenization approaches takes into consideration the interfacial thermal resistance for the estimation of thermal properties of composites. These homogenization techniques are an approximate method and are usually not accurate as atomistic simulation techniques. For modeling interfacial thermal effects, the interfacial thermal resistance ( $R_k$ ) can be considered as a layer around the nanotube offering a higher resistance to the flow of thermal energy as shown in Fig. 4.

#### 3.1 Wakashima-Tsukamoto estimate

The Wakashima-Tsukamoto estimate is widely used in the estimation of the effective thermal conductivity of composite structures especially for predicting the overall effective properties of composites and functionally graded materials (Li and Wang 2005, Yokota *et al.* 2003). The WT estimate is based on the Eshelby’s Equivalent Inclusion (EEI) principle and further details of the EEI principle can be found in Mura (1997). In the WT estimate, the effective thermal conductivities of a dual phase composite material are given by:

$$K_{eff} = K_m + \frac{v_p \{A^0\} (K_p - K_m)}{(1 - v_p) + \{A^0\} v_p} \tag{3}$$

where  $K_{eff}$  is the effective thermal conductivity of the composite material,  $3\{A^0\} = \sum_{k=1}^3 \frac{K_m}{K_m + S^{(k)}(K_p - K_m)}$ .  $K_m$  &  $K_p$  are the thermal conductivities of the matrix phase and of the fiber phase which has a volume fraction  $v_p$ ,  $\{A^0\}$  are the strain concentration factors due to the inclusion and  $S^k$  is the Eshelby tensor. In the WK estimate, the discrete phases are represented by groups of ellipsoidal particles of the same shape (Mura 1997) and the Eshelby tensor for cylindrical fiber is used in this paper. One of the major drawbacks of this method is that the effect of interfacial thermal resistance is neglected.

### 3.2 Hashin-Shtrikman (H-S) bounds

The Hashin-Shtrikman (H-S) bounds for thermal conductivity of a two-phase material is given in Eqs. (4) and (5) Readers may refer to standard literature on micromechanical analysis (Mura 1997) for a detailed description of the HS bounds. In the HS estimates the bounds are derived from the thermal properties and volume fractions of the individual phases for homogeneous, isotropic, two-phase materials.

$$K_{lower} = K_m + 3v_f(3(K_p - K_m)^{-1} + (1 - v_f)K_m^{-1})^{-1} \quad (4)$$

$$K_{upper} = K_p + 3(1 - v_f)(3(K_m - K_p)^{-1} + v_fK_m^{-1})^{-1} \quad (5)$$

where  $K_{lower}$  and  $K_{upper}$  are the H-S lower and upper bounds respectively.

### 3.3 Maxwell-Garnett type effective medium theory

This theory is valid for small volume fractions of fiber materials where the thermal conductivity of the fiber phase is assumed to be larger than that of the matrix phase. The effective thermal conductivity of a nanotube composite system is given by (Nan *et al.* 2004, Nan *et al.* 2003).

$$K_{eff} = K_m(3 + v_f(\beta_x + \beta_z))(2 - v_f\beta_x)^{-1} \quad (6)$$

with,  $\beta_x = 2(K_{11}^c - K_m)(K_{11}^c + K_m)^{-1}$  and  $\beta_z = (K_{33}^c - K_m)K_m^{-1}$  and  $v_f$  is the volume fraction of the nanotube fiber phase.  $K_m$  and  $K_c$  are the thermal conductivities of the matrix phase and the fiber phase respectively,  $K_{11}^c$  and  $K_{33}^c$  are the equivalent thermal conductivities along transverse and longitudinal axes of a composite unit cell as seen in Fig. 4.

$$K_{33}^c = K_c \left(1 + K_c \frac{2R_K}{L}\right)^{-1} \quad (7)$$

$$K_{11}^c = K_c \left(1 + K_c \frac{2R_K}{d}\right)^{-1} \quad (8)$$

### 3.4 Bruggeman Effective Medium Theory

Bruggeman's EMT takes into consideration the effective thermal resistance and the average polarization theory for the estimation of the effective thermal conductivity (Gao *et al.* 2007, Xue 2005, 2006). According to this theory, the effective thermal conductance is related to the thermal resistance of the matrix and the fiber phase material and its volume fraction(Gao *et al.* 2007, Xue 2006). The effective thermal conductance of the composite material is given by Eq. (9).

$$\frac{1}{9} \left[ \frac{K_{eff} - K_{c,x}}{K_{eff} + L_x(K_{c,x} - K_{eff})} + 4 \frac{K_{eff} - K_{c,y}}{2K_{eff} + (1 - L_x)(K_{c,y} - K_{eff})} \right] \left( \frac{K_m - 2K_{eff}}{K_m - K_{eff}} \right) = 1 - \frac{1}{v_f} \quad (9)$$

where, the aspect ratio of the nanotube is  $P = a/c$ , and  $L_j$  is the depolarization factor,  $K_m$  is the

thermal conductivity of matrix phase,  $K_{c,j} = K_p(1 + QR_K L_j K_p)^{-1}$  is the thermal conductivity of the fiber along  $j$ -axis,  $R_K = \lim_{\delta \rightarrow \infty, K_s \rightarrow 0} \delta / K_s$  is the interfacial thermal resistance obtained from molecular dynamic simulations and  $Q = \frac{(2a + c)}{ac}$ .

$$L_x = 2(P^2 - 1)^{-3/2} \left[ P \ln \frac{P + \sqrt{P^2 - 1}}{P - \sqrt{P^2 - 1}} - 2\sqrt{P^2 - 1} \right]; \quad L_x = 1 - 2L_y \text{ \& } L_z = L_y \quad (10)$$

#### 4. Results and discussion

From the simulations it can be seen that the temperature profile follows an exponential order as shown in Fig. 5 for single walled nanotubes. The cooling profile for double walled nanotubes

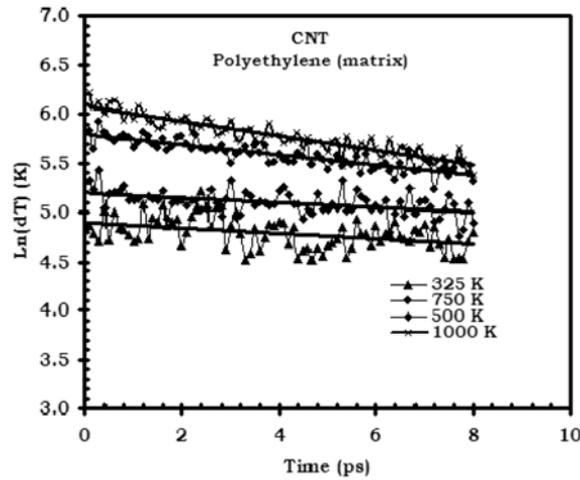


Fig. 5 Cooling profile of single walled nanotube in LDPE

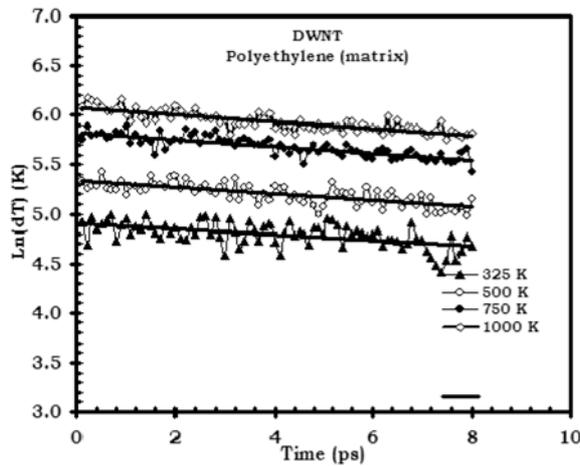


Fig. 6 Cooling profile of double walled nanotube in LDPE

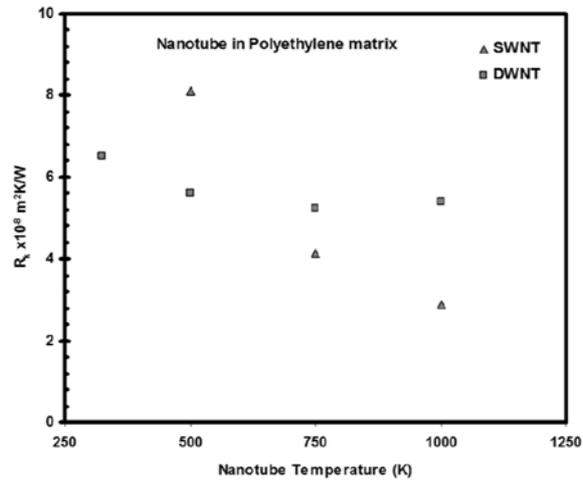


Fig. 7 Interface thermal resistance values of single and double walled nanotube heated to various target temperatures.

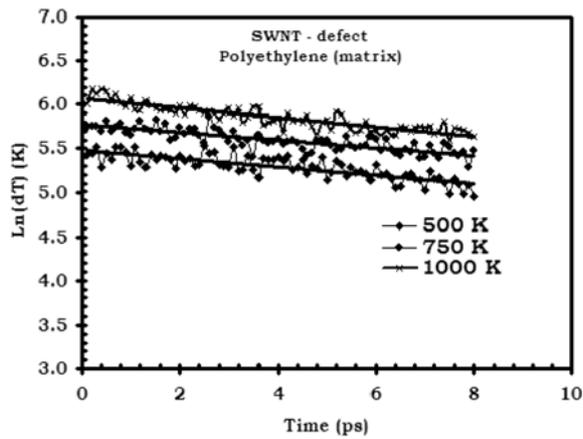


Fig. 8 Cooling profile of single walled nanotube in LDPE with 1-Stone-Wales defect

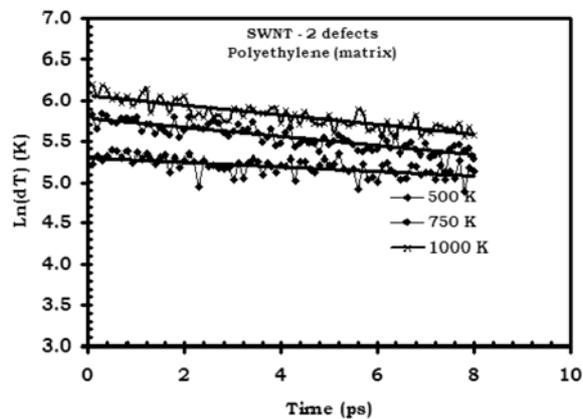


Fig. 9 Cooling profile of single walled nanotube in LDPE with 2-Stone-Wales defect

embedded in LDPE is shown in Fig. 6 and the variation of the estimated interfacial thermal resistance for pristine and defective nanotubes with Stone-Wales defects (Fig. 1b) at various target temperatures are shown in Figs. 7, 8 and 9. The effect of the Stone-Wales defect on the interfacial thermal resistance is shown in Fig. 10. The average interfacial thermal resistance of single walled nanotube embedded in LDPE was found to be  $5.05 \times 10^{-8} \text{ m}^2\text{K/W}$ .

This value of the interfacial thermal resistance was found to be well within the experimental and analytical studies. The effect of the defects in single walled nanotubes was found to decrease the interfacial thermal resistance values as  $3.85 \times 10^{-8} \text{ m}^2\text{K/W}$  and  $4.42 \times 10^{-8} \text{ m}^2\text{K/W}$  for one and two defects respectively. The thermal resistance values obtained from the simulations are now used in

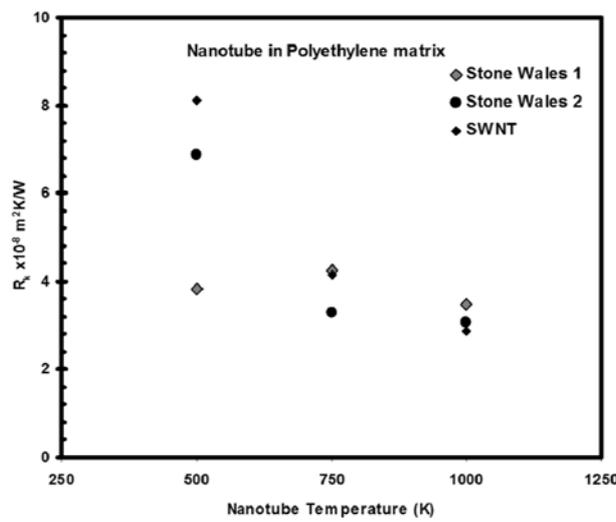


Fig. 10 Interface thermal resistance values of defective single walled nanotube heated to various target temperatures

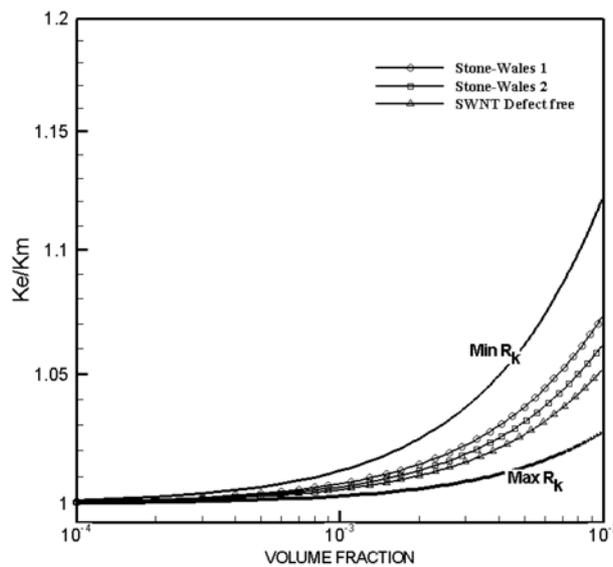


Fig. 11 Effective thermal coefficient of single walled nanotube in LDPE

the estimation of the mesoscale thermal conductivity of nanocomposites by using the various effective medium theories and are compared with the micromechanical methods.

Thermal conductivities of the nanotube and the polymer composite systems are used for the estimation of the overall effective conductivity. The conductivity of single walled nanotube was taken as 6000 W/mK and that of polyethylene (LDPE) is taken as 0.33 W/mK. Using the Maxwell-Garnett type effective medium approach, the effective thermal conductivities lies between the thermal conductivities from the maximum and minimum reported values of the interfacial thermal resistances (Huxtable *et al.* 2003, Xue 2006) as shown in Fig. 11. The effective thermal conductivity for 5% fiber volume fraction with varying interfacial thermal resistance, shows a nonlinear dependence on the change in the thermal conductivity of the nanotube composite structure (Nan *et al.* 2004) as shown in Fig. 12.

Using the Bruggeman's EMT, HS bounds, and the WT estimates, the effective thermal

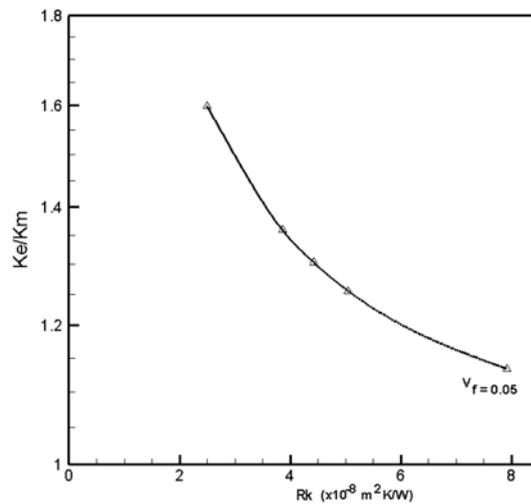


Fig. 12 Variation of effective thermal coefficient with interfacial thermal resistance values for volume fraction 0.05

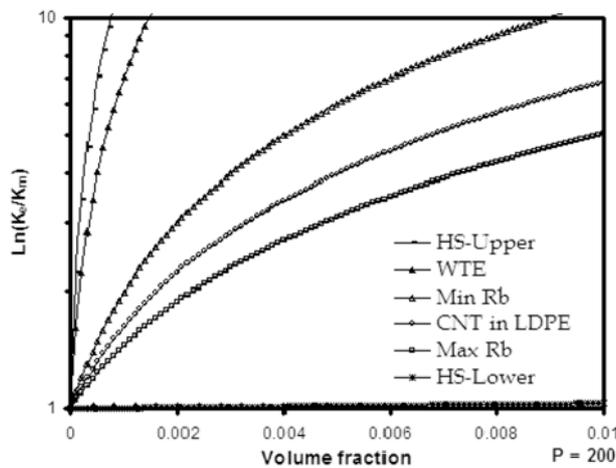


Fig. 13 Effective thermal coefficient of single walled nanotube in LDPE with bounds

conductivities for various interfacial thermal resistances is also found to give a good estimate of the thermal conductivities when compared with maximum and minimum reported values of interfacial thermal resistances reported in literature as seen in Figs. 13 and 14. For double walled nanotubes based composite systems, the effective thermal conductivities are shown in Fig. 13 using the Maxwell-Garnett type effective medium approach for various fiber phase volume fractions and the thermal conductivity of multiwalled nanotubes is taken as 3000 W/mK from literature (Nan *et al.* 2004). It should be noted that the interfacial thermal resistance obtained are dependent on the length of the nanotube and also on the type of potential function used in the molecular dynamic simulations.

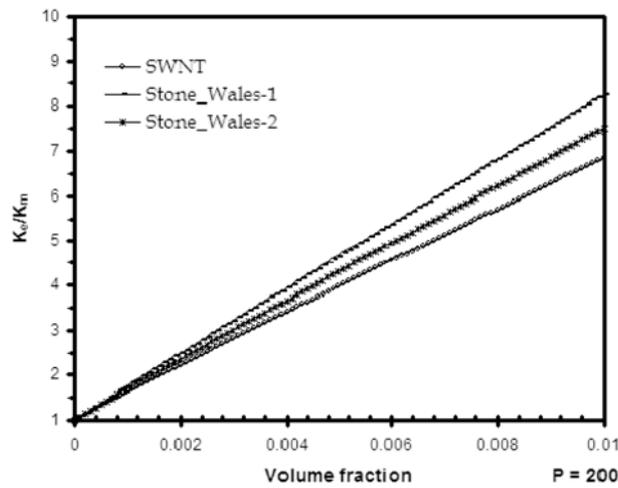


Fig. 14 Effective thermal coefficient of pristine and defective single walled nanotube in LDPE

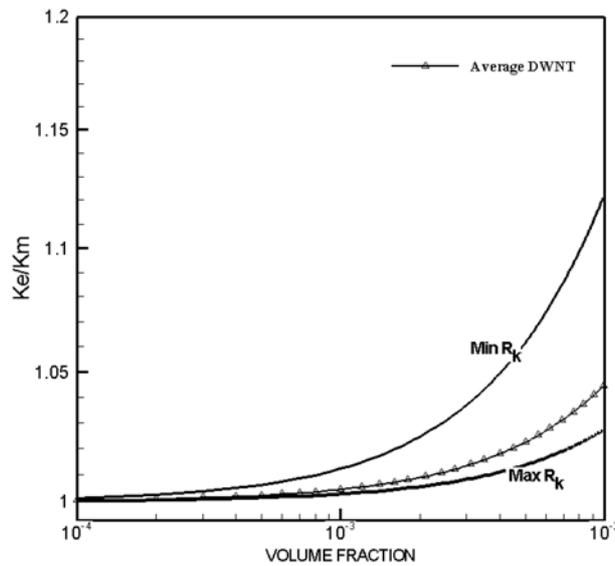


Fig. 15 Effective thermal coefficient of double walled nanotube in LDPE

## 5. Conclusions

Thermal conductivity of pristine and defective nanotube-polymer nanocomposite system is studied in this paper. The interfacial thermal resistance for various nanotubes was obtained by molecular dynamic simulations and it was found that the development of defects in nanotubes significantly affects the interfacial thermal resistance: larger the density of defects greater is the effect on the interfacial thermal resistance. The interfacial thermal resistance values from the analysis are also found to be within the values obtained from literature for the length of the nanotube used in the analysis. The estimated interfacial thermal resistance was subsequently used in various effective medium theories to ascertain the effect on the overall thermal conductance of the composite system and it was found that the effective conductivities are bounded by the various micromechanical bounds.

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