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EFFECT OF NANOTUBE THICKNESS ON THE EQUIVALENT THERMAL CONDUCTIVITY OF NANO-COMPOSITES

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In this paper, a numerical simulation has been carried out to study the effect of nanotube thickness on the equivalent thermal conductivity of the composite. Square representative volume element containing single nanotube has been used a model problem to evaluate the thermal conductivity of the composite. The equivalent thermal conductivity of the composite has been evaluated by element free Galerkin method using continuum mechanics approach. The results have been obtained for few typical values of nanotube lengths. The present computations show that for small length nanotubes, thickness does not have much effect on the effective thermal conductivity of the composite, whereas for long nanotubes, thickness has a significant effect on the effective conductivity of the composite.

Keywords: Carbon nanotube; nano-composites; nanotube thickness; thermal conductivity, and element free Galerkin method

1. Introduction

In last decade, carbon nanotubes (CNTs) have attracted many researchers towards the field of nanotechnology due to their excellent physical, mechanical, electronic, and thermal properties. Now days, CNTs became a major filed of research for scientists and researchers due to their remarkable properties. Many researchers believe that the reinforcement of CNTs in polymer matrix may provide us an entirely new class of composite materials [1-9]. Carbon nanotubes may be single walled (SWNT), double walled (DWNT), and multi-walled (MWNT) depending upon their processing and production methodology.

Heat conduction plays a fundamentally critical role in the performance and stability of nano/micro devices. Therefore, the study of the thermal properties of nano-composites becomes increasing important with the reduction of device size. In recent years, few numerical simulations were carried to predict the thermal properties of nano-composites out using continuum mechanics approach [10-13]. Zhang et al. [10-11] used the meshless hybrid boundary node method (hybrid BNM) for the heat conduction analysis of CNT based nano-composites. They used both multi-domain and simplified approaches to predict the thermal properties of nano-composites, and also coupled their method with fast multipole method to solve large scale problems. Nishimura and Liu [12] applied the boundary integral equation (BIE) method for the thermal analysis of CNT based nano-composites. They analyzed a heat conduction problems in two-dimensional infinite domain embedded with many rigid inclusions with the help of a fast multipole boundary element method. Singh et al. [13] applied the element free Galerkin method to evaluate the equivalent thermal conductivity of CNT based composites. They used both simplified and multi-domain approaches for the numerical simulation of CNT based composites, and found that the thermal conductivity of the composite is function of RVE as well as nanotube dimensions.

So far in continuum mechanics based numerical simulations, thickness of nanotube has been taken as constant to evaluate the thermal properties. Therefore, in the present work, the effect of nanotube thickness on the equivalent thermal conductivity of the composites has been studied in detail for few typical values of nanotube lengths. The meshless element free Galerkin method has been used a numerical tool to evaluate the thermal properties. A nanoscale square representative volume element (square RVE) containing single CNT has been taken to evaluate the thermal properties of the composites using continuum mechanics approach. Penalty method has been used to enforce the essential boundary conditions.

2. Review of EFG Method

The element free Galerkin (EFG) method requires moving least square (MLS) approximations for the discretization of the governing equation. These MLS approximation function consist of three components: a weight function associated with each node, a basis function, and a set of constant coefficients that depends on node position. Using MLS approximation scheme, an unknown function of temperature $T(\mathbf{x})$ is approximated as $T^h(\mathbf{x})$ [13].

$$T^h(\mathbf{x}) = \sum_{I=1}^{n} \Phi_I(\mathbf{x}) T_I = \mathbf{\Phi}(\mathbf{x})\mathbf{T} \tag{1}$$

where $\mathbf{x}^T = [x \quad y \quad z]$, T_I are the nodal parameters and $\Phi_I(\mathbf{x})$ is the shape function, which is defined as

$$\Phi_I(\mathbf{x}) = \sum_{j=1}^{m} p_j(\mathbf{x})(\mathbf{A}^{-1}(\mathbf{x})\mathbf{B}(\mathbf{x}))_{jI} = \mathbf{p}^T \mathbf{A}^{-1} \mathbf{B}_I \tag{2a}$$

where

$$\mathbf{A} = \sum_{I=1}^{n} w(\mathbf{x}-\mathbf{x}_I)\mathbf{p}(\mathbf{x}_I)\mathbf{p}^T(\mathbf{x}_I) \tag{2b}$$

$$\mathbf{B}(\mathbf{x}) = [w(\mathbf{x}-\mathbf{x}_1)\mathbf{p}(\mathbf{x}_1),............w(\mathbf{x}-\mathbf{x}_n)\mathbf{p}(\mathbf{x}_n)] \tag{2c}$$

The rational weight function [14] has been used in this work, which is given as

$$w(s) = \begin{Bmatrix} \dfrac{1}{s^{\bar{n}}+C} & 0 \le s \le 1 \\ 0 & s > 1 \end{Bmatrix} \tag{3}$$

where $2 \le \bar{n} \le 7$, $0.01 \le C \le 0.1$, $s = \dfrac{\| \mathbf{x} - \mathbf{x}_I \|}{d_{mI}}$ is the normalized radius, $d_{mI} = d_{\max} c_I$ and $d_{\max}$ = scaling parameter (for complete details of EFG method, refer to article by Belytschko et al. [15]).

3. Numerical Implementation

A model containing single CNT inside square RVE has been taken to study the effect of nanotube thickness on the equivalent thermal conductivity of the composite. The top and bottom surfaces of RVE are subjected to constant temperatures, while other surfaces are kept insulated. The governing Laplace equation in Cartesian coordinate system is given as

$$k\nabla^2 T = 0 \tag{4a}$$

The essential boundary conditions and the continuity requirements at the interface of matrix and CNT are given as follows

at $z=0$, $T = T_1$ (4b)

at $z=L$, $T=T_2$ (4c)

Continuity of temperature, $T|_m = T|_c$ (4d)

Continuity of normal heat flux, $q_n|_m = q_n|_c$ (4e)

where $\nabla^T = \begin{bmatrix} \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \end{bmatrix}$

The weighted integral form of Eq. (4a) is given as

$$\sum_{i=m,c} \int_{V_i} \bar{w}\{k_i \nabla^2 T\} dV = 0 \tag{5}$$

Using divergence theorem, the weak form of Eq. (5) is obtained as

$$\sum_{i=m,c} \int_{V_i} \{k_i (\nabla^T w)\nabla T\} dV = 0 \tag{6}$$

From Eq. (6), the functional $I(T)$ can be obtained as

$$I(T) = \sum_{i=m,c} \int_{V_i} \left\{\frac{1}{2} k_i (\nabla^T T)\nabla T\right\} dV \tag{7}$$

Enforcing essential boundary conditions using Lagrange multiplier method, the functional $I^*(T)$ is obtained as

$$I^*(T) = \sum_{i=m,c} \int_{V_i} \left\{\frac{1}{2} k_i (\nabla^T T)\nabla T\right\} dV + \frac{\alpha}{2}\int_{S_1} (T-T_1)^2 dS + \frac{\alpha}{2}\int_{S_2} (T-T_2)^2 dS \tag{8}$$

Taking variation i.e. $\delta I^*(T)$ of Eq. (8), it reduces to

$$\delta I^*(T) = \sum_{i=m,c} \int_{V_i} \{k_i (\nabla^T T)\delta\nabla T\} dV + \alpha \int_{S_1} (T-T_1)\delta T\, dS + \alpha \int_{S_2} (T-T_2)\delta T\, dS \tag{9}$$

Since $\delta I^*(T) = 0$ and δT is arbitrary in Eq. (9), hence a following set of linear equations is obtained using Eq. (1)

$$[\mathbf{K}]\{\mathbf{T}\} = \{\mathbf{f}\} \tag{10a}$$

where

$$K_{IJ} = \sum_{i=m,c} \int_{V_i} \begin{bmatrix} \Phi_{I,x} \\ \Phi_{I,y} \\ \Phi_{I,z} \end{bmatrix}^T \begin{bmatrix} k_i & 0 & 0 \\ 0 & k_i & 0 \\ 0 & 0 & k_i \end{bmatrix} \begin{bmatrix} \Phi_{J,x} \\ \Phi_{J,y} \\ \Phi_{J,z} \end{bmatrix} dV + \int_{S_1} \alpha \Phi_I^T \Phi_J \, dS + \int_{S_2} \alpha \Phi_I^T \Phi_J \, dS \tag{10b}$$

$$f_I = \int_{S_1} \alpha T_1 \Phi_I \, dS + \int_{S_2} \alpha T_2 \Phi_I \, dS \tag{10c}$$

4. Numerical Results and Discussion

In this section, a model problem has been solved by element free Galerkin method to study the effect of nanotube thickness on the equivalent thermal conductivity of the composite. A square representative volume element containing single nanotube is shown in Fig. 1. Nanotube is placed symmetrically at the center of RVE such that the axis of RVE is coinciding with the axis of nanotube. The top and bottom surfaces of RVE are maintained at two different constant temperatures, and other surfaces are kept insulated. The data required for this study is tabulated in Table 1. Penalty approach has been used to enforce the essential boundary conditions. Assuming material properties as homogeneous, isotropic and independent of temperature, the equivalent thermal conductivity of the composite has been evaluated as

$$k_e = -\frac{q_n L}{\Delta T} \tag{11}$$

where k_e denotes the equivalent thermal conductivity of the composite, L is the length of RVE, q_n is normal heat flux density and ΔT is the temperature difference between two ends of RVE.

The volume fraction of nanotube has been calculated by the following expression

$$v = \left(\frac{V_c}{V_c + V_m}\right) \tag{12}$$

where v is the volume fraction of CNT in composite, V_c is the volume of CNT including cavity, and V_m is the volume of polymer matrix.

Various nanotube thickness values i.e. from 0.5 nm to 8 nm have been chosen to study the effect of nanotube thickness on the equivalent thermal conductivity of the composite. Fig. 1 shows the effect of nanotube thickness (t) on the equivalent thermal conductivity (k_e) of the composites for L_c = 300 nm. From Fig. 1, it can be seen that initially there is small increase in the equivalent thermal conductivity of the composite with the increase of nanotube thickness after that k_e becomes almost constant with the further increase of nanotube thickness. The effect of nanotube thickness on the equivalent thermal conductivity of the composite has also been presented in Fig. 2 for L_c = 500 nm and in Fig. 3 for L_c = 800 nm. From the results presented in Fig. 1, Fig. 2 and Fig. 3, it has been noticed that for small length CNTs, nanotube thickness does not have much effect on the overall thermal conductivity of the composite, but for long CNTs, nanotube thickness has a significant effect on the overall thermal conductivity of the composite.

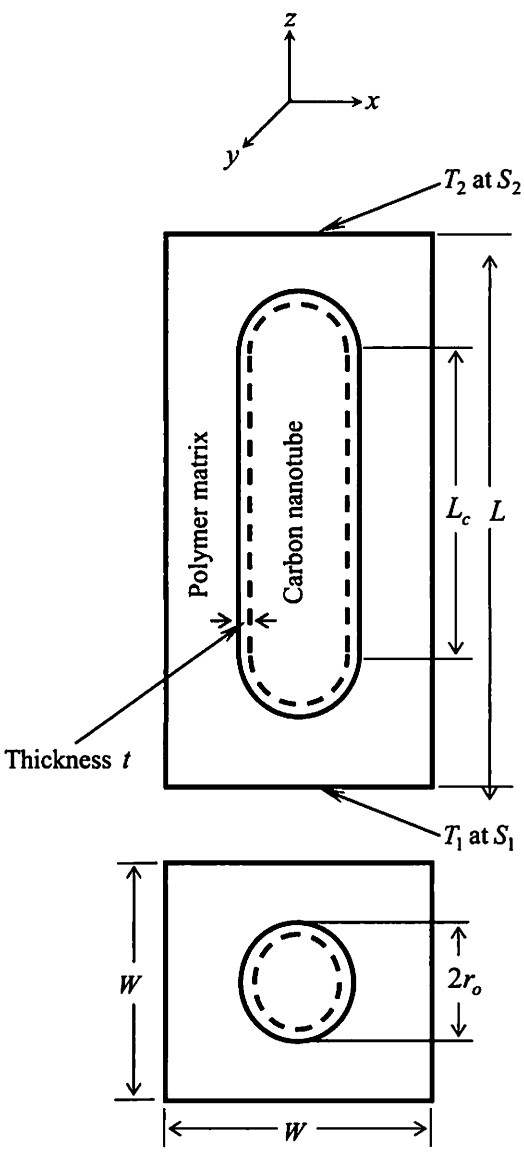

Fig. 1: Nano scale representation of a nano-composite

Table 1: Data for CNT based composite problem

Parameter	Value of parameter
RVE length, L	1000 nm
RVE cross-sectional dimension, W	60 nm
Nanotube length, L_c	300, 500 & 800 nm
Nanotube outer radius, r_o	10 nm
Nanotube thickness, t	0.5 - 8 nm
Thermal conductivity of matrix, k_m	0.37 W/m-K
Thermal conductivity of CNT, k_c	3000 W/m-K
Temperature at S_1, T_1	300 K
Temperature at S_2, T_2	100 K

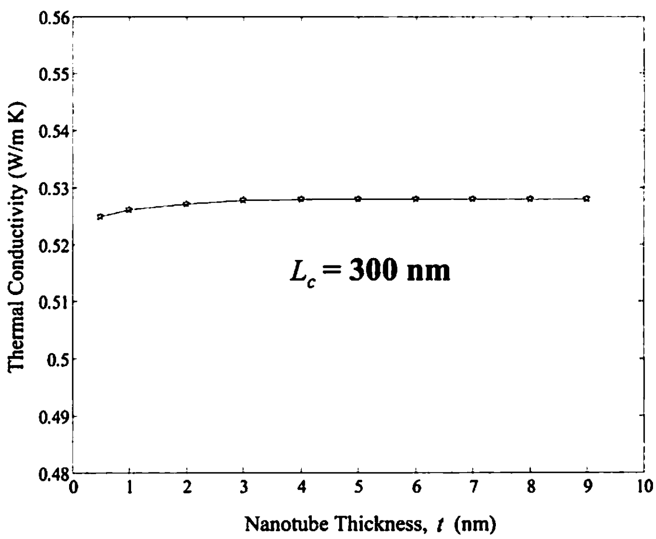

Fig. 2: Variation of equivalent thermal conductivity (k_e) with nanotube thickness (t) for L_c = 300 nm

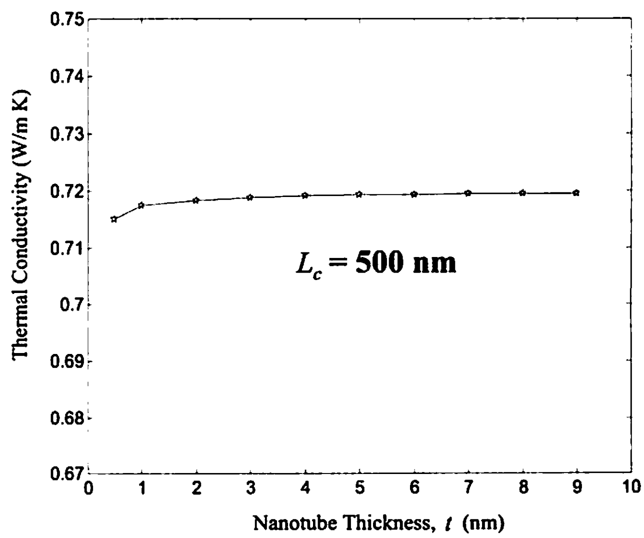

Fig. 3: Variation of equivalent thermal conductivity (k_e) with nanotube thickness (t) for L_c = 500 nm

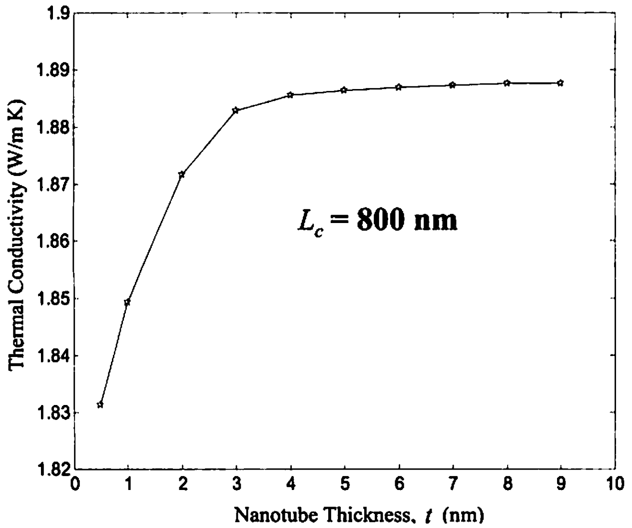

Fig. 4: Variation of equivalent thermal conductivity (k_e) with nanotube thickness (t) for L_c = 800 nm

5. Conclusions

In the present work, the effect of nanotube thickness on the equivalent thermal conductivity of the composite was studied in detail by element free Galerkin method. The thermal conductivity of composite was evaluated using continuum mechanics approach. The results were obtained by penalty approach for a model composite problem. The numerical simulations show that the nanotube thickness does not have much effect on the effective thermal conductivity of the composite for small length nanotubes but for long nanotubes, thickness has a significant effect on the overall thermal conductivity of the composite. On the basis of these simulations, it can also be concluded that small length multi-walled nanotubes can be considered as a solid for performing the numerical simulations of CNT based composites.

Notations

k_c thermal conductivity of nanotube, W/m K
k_e equivalent thermal conductivity of composite, W/m K
k_m thermal conductivity of matrix, W/m K
L length of cylindrical RVE, nm
L_c nanotube length, nm
m number of terms in basis
n number of nodes in the domain of influence
$p_j(\mathbf{x})$ monomial basis function
q_n normal heat flux, W/m^2
r_o nanotube outer radius, nm
t nanotube thickness, nm
$T^h(\mathbf{r})$ MLS approximation function for temperature
w weight function used in MLS approximation
$\overline{w}$ weighting function used in weighted integral form
V computational domain
$\Phi_I(\mathbf{r})$ shape function
α penalty parameter

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