HEAT CONDUCTION ANALYSIS OF CNT BASED COMPOSITES WITH TEMPERATURE DEPENDENT MATERIAL PROPERTIES

Masataka Tanaka

O Indra Vir Singh

Morinobu Endo

Indra Vir Singh, Shinshu University, 4-17-1 Wakasato, Nagano, 380-8553
 Masataka Tanaka, Shinshu University, 4-17-1 Wakasato, Nagano 380-8553
 Morinobu Endo, Shinshu University, 4-17-1 Wakasato, Nagano 380-8553

Key Words: Carbon nanotube, nano-composites, nonlinear, temperature dependent thermal conductivity, meshless, EFG method

1. Introduction

The discovery of carbon nanotubes has attracted the wide attention of various scientists and researchers towards the field of nanotechnology. Numerous studies showed that carbon nanotubes exhibit exceptional mechanical, thermal and electronic properties over other known materials and hold substantial promise as super-fibers for composite materials. The rapid advance in the synthesis of CNTs has made it possible to produce CNTs-based composites. Recent studies reveal that CNTs have anomalously high thermal conductivity. It is expected that the nanotube suspensions can enhance the thermal conductivity, hence can improve the thermal performance of the composites. In last decade, lot of work has been done on the CNT based composites [1-2]. Still, much work is needed before the potential of nanotube based composites is fully realized.

In the present work, nonlinear heat conduction analysis of CNT based composites have been carried out using element free Galerkin method. Thermal conductivity of nanotube is assumed to vary linearly with the temperature. A successive substitution scheme (Picard method) has been used to obtain the solution of nonlinear equations. Cylindrical representative volume element (cylindrical RVE) has been taken to evaluate the thermal properties of the composite.

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 approximations 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 $T(\mathbf{r})$ is approximated as $T^h(\mathbf{r})$ [3].

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

where, T_I are the nodal parameters and $\Phi_I(\mathbf{r})$ is the shape function, (for complete details of EFG method, refer to article by Belytschko et al. [4]).

3. Numerical Implementation

To evaluate the nonlinear thermal properties of CNT based composites, a cylindrical representative volume element (RVE) has been taken containing single CNT inside it (as shown in Fig.1). CNT has been placed at the center of RVE such that the axis of CNT overlaps with the axis of RVE. Both ends of RVE are maintained at two different constant temperatures and outer surface has been kept insulated. For this axisymmetric heat transfer problem, the governing steady state heat conduction equation in cylindrical coordinate system is given as

$$k \frac{\partial T}{\partial r^2} + \frac{k}{r} \frac{\partial T}{\partial r} + k \frac{\partial T}{\partial z} = 0 \quad (2a)$$

along with the following essential boundary conditions and compatibility condition at the interface of matrix and CNT

$$\text{at } z=0, \quad T = T_L \quad (2b)$$

$$\text{at } z=L, \quad T = T_R \quad (2c)$$

$$\text{at interface} \quad \bar{q}_m = \bar{q}_c \quad (2d)$$

where, $\bar{q}_m$ and $\bar{q}_c$ are the value of heat fluxes at the interface

Fig. 1: Nano scale representation of a composite problem

From Eq. (2), the functional $I(T)$ is obtained as

$$I(T) = \pi \int_{\Omega_c} k_c(T) \left[\left(\frac{\partial T}{\partial r} \right)^2 + \left(\frac{\partial T}{\partial z} \right)^2 \right] r dr dz + \pi \int_{\Omega_m} k_m \left[\left(\frac{\partial T}{\partial r} \right)^2 + \left(\frac{\partial T}{\partial z} \right)^2 \right] r dr dz \quad (3)$$

where, $k_c(T) = k_o(1 + \beta T)$, k_c and k_m are the values of thermal conductivities for the nanotube and polyimide matrix respectively.

Enforcing essential boundary conditions using penalty method, the functional $I^*(T)$ is modified as

$$I^*(T) = \pi \int_{\Omega_c} k_c(T) \left[\left(\frac{\partial T}{\partial r} \right)^2 + \left(\frac{\partial T}{\partial z} \right)^2 \right] r dr dz + \frac{\alpha}{2} \int_{\Gamma_1} (T - T_L)^2 d\Gamma + \pi \int_{\Omega_m} k_m \left[\left(\frac{\partial T}{\partial r} \right)^2 + \left(\frac{\partial T}{\partial z} \right)^2 \right] r dr dz + \frac{\alpha}{2} \int_{\Gamma_2} (T - T_R)^2 d\Gamma \quad (4)$$

Taking variation i.e. $\delta I^*(T)$ of Eq. (4), a following set of nonlinear equations is obtained using Eq. (1)

$$[\mathbf{K}(\mathbf{T})][\mathbf{T}] = \{\mathbf{F}\} \quad (5a)$$

where,

$$K_{IJ} = 2\pi \int_{\Omega_c} \begin{bmatrix} \Phi_{I,r} \\ \Phi_{I,z} \end{bmatrix}^T \begin{bmatrix} k_c(T) & 0 \\ 0 & k_c(T) \end{bmatrix} \begin{bmatrix} \Phi_{J,r} \\ \Phi_{J,z} \end{bmatrix} r dr dz + \alpha \int_{\Gamma} \Phi_I^T \Phi_J d\Gamma \quad (5b)$$

$$+ 2\pi \int_{\Omega_m} \begin{bmatrix} \Phi_{I,r} \\ \Phi_{I,z} \end{bmatrix}^T \begin{bmatrix} k_m & 0 \\ 0 & k_m \end{bmatrix} \begin{bmatrix} \Phi_{J,r} \\ \Phi_{J,z} \end{bmatrix} r dr dz + \alpha \int_{\Gamma_s} \Phi_I^T \Phi_J d\Gamma$$

$$F_I = \alpha \int_{\Gamma_l} T_L \Phi_I d\Gamma + \alpha \int_{\Gamma_r} T_R \Phi_I d\Gamma \quad (5c)$$

Eq. (5a) represents a system of nonlinear algebraic equations, which will be linearized first to obtain a set of linear equations. Picard scheme (successive substitution scheme) has been used to solve the nonlinear equations

$$[\mathbf{K}(\mathbf{T}^N)][\mathbf{T}^{N+1}] = \{\mathbf{F}\} \quad (6)$$

By evaluating the coefficient matrix $[\mathbf{K}]$ from previous iteration, the system of nonlinear equations is linearized and solved by standard matrix solution technique. The solution obtained from the previous iteration is then used to evaluate the coefficient matrix for the next iteration and this process is continued until the root mean square value of the difference between the solution vectors at two consecutive iterations is reduced to a value less than a prescribed tolerance ϵ , which is calculated by the following expression:

$$\frac{([\mathbf{T}]^{N+1} - [\mathbf{T}]^N)^T ([\mathbf{T}]^{N+1} - [\mathbf{T}]^N)}{([\mathbf{T}]^{N+1})^T ([\mathbf{T}]^{N+1})} < \epsilon \quad (7)$$

where, N is the iteration number and $\epsilon = 10^{-4}$.

4. Results and Discussion

In this section, a model heat conduction problem has been solved to evaluate the thermal conductivity of the composite using element free Galerkin method. The thermal conductivity (k_c) of the nanotube is assumed to be vary linearly with temperature whereas the thermal conductivity (k_m) of polymer matrix (polyimide) is taken as constant. A nanoscale cylindrical representative volume element containing single nanotube is shown in Fig. 1 along with the dimensions. Carbon nanotube is placed symmetrically at the center of RVE such that the axes of both RVE and CNT are coinciding with each other. Two ends of cylindrical RVE are maintained at two different constant temperatures and outer cylindrical surface is kept flux free. The following data has been chosen for the analysis nano-composite:

$L = 100$ nm, $r_o = 5$ nm, $t = 0.34$ nm, $T_L = 300$ K, $T_R = 100$ K, $k_m = 0.12$ W/m-K, $k_o = 3000$ W/m-K, $\beta = 10^{-3}$ K $^{-1}$ and 10^{-2} K $^{-1}$

The equivalent thermal conductivity (k_e) of the composite has been evaluated by taking constant and temperature dependent thermal conductivities of the nanotube. A successive substitution approach knows as Picard method has been used to obtain the solution of nonlinear equations. The solution of a system of nonlinear equations is achieved in the couple of iterations by Picard method. Four points Gaussian quadrature has been used to integrate Eqs. (5b) and (5c). The EFG results have been obtained using uniform nodal distribution scheme for 3111 nodes. Various values of CNT length (L_c) i.e. from 25 nm to 75 nm have been chosen to study the effect of CNT length on the equivalent thermal conductivity of the composite. Fig. 2 shows a variation of equivalent thermal conductivity of the composite with CNT length for constant and temperature dependent nanotube thermal conductivities. The addition of 5.5% (by volume) of CNT with constant thermal conductivity increases the thermal conductivity of the polymer matrix by 41.5% whereas in case of temperature dependent nanotube thermal conductivity, the same amount of CNT addition increases the thermal conductivity of the polymer

matrix by 41.5% and 41.7% for $\beta = 10^{-3}$ K $^{-1}$ and $\beta = 10^{-2}$ K $^{-1}$ respectively. The addition of 14.2% (by volume) of CNT with constant thermal conductivity results in an increase of 342.5%, in the thermal conductivity of the polymer matrix, whereas same amount of CNT with temperature dependent thermal conductivity increases the thermal conductivity of the polymer matrix by 344.0% and 349.9% for $\beta = 10^{-3}$ K $^{-1}$ and $\beta = 10^{-2}$ K $^{-1}$ respectively. From Fig. 2, it is also observed that the temperature dependent thermal conductivity of nanotube has small effect on the equivalent thermal conductivity of the composite.

Fig. 2: Variation of equivalent thermal conductivity with nanotube length

5. Conclusions

In this work, nonlinear thermal analysis of carbon nanotube based composites was carried out by element free Galerkin method. The thermal conductivity of the nanotube was taken as function of temperature and was assumed to vary linearly with the temperature. Picard method was used to obtain the solution of nonlinear equations. Present simulation shows that the addition of 14.2% (by volume) of CNT with constant thermal conductivity results in an increase of 342.5%, in the thermal conductivity of the polymer matrix, whereas the same amount of CNT addition with temperature dependent thermal conductivity increases the thermal conductivity of the polymer matrix by 344% and 349.9% for $\beta = 10^{-3}$ K $^{-1}$ and $\beta = 10^{-2}$ K $^{-1}$ respectively. The analysis shows that temperature dependent thermal conductivity does not have much effect on the equivalent thermal conductivity of the composite.

Acknowledgement

This work was supported by the CLUSTER of Ministry of Education, Culture, Sports, Science and Technology, Japan.

References

1. P. J. F Harris, Carbon nanotube composites, *International Materials Reviews*, vol. 49, pp. 31-43, 2004.
2. R. Khare, S. Bose, Carbon nanotube based composites-a review, *Journal of Minerals & Materials Characterization & Engineering*, vol. 4, pp 31-46, 2005.
3. I. V. Singh, A numerical solution of composite heat transfer problems using meshless method, *International Journal of Heat and Mass Transfer*, vol. 47, pp. 2123-2138, 2004.
4. T. Belytschko, Y. Y. Lu and L. Gu, Element free Galerkin methods, *International Journal for Numerical Methods in Engineering*, vol. 37, pp. 229-256, 1994.