HEAT CONDUCTION IN CNT COMPOSITES USING A THREE-PHASE MODEL

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Abstract

Heat conduction in CNT composites is analyzed using three-phase model. A set of permissible functions are derived that satisfy the temperature and heat flux continuity condition across the interface using a computer algebra system. The temperature field is expressed by a linear combination of the permissible functions semi-analytically. An example is shown to depict the temperature field subject to uniform heat flux at infinity. Parametric study is possible with the CNT aspect ratio, the size of CNT and the thermal conductivity of each phase.

1 Introduction

CNT based composites are futuristic materials with high strength and high thermal/electrical conductivities [1]. However, despite its promising improvement over conventional FRP composites, experimental results show that heat conduction in CNT composites is disappointedly smaller than predicted values from conventional micromechanics theory. This difference is believed to be due to several factors such as the presence of thermal barriers between CNTs and the matrix or misaligned orientation of CNTs in the matrix phase. Because of the difficulty in analysis, no clear authoritative explanation has been established. The present paper attempts to investigate heat conduction in CNT composites using a three-phase model that satisfies the continuity conditions of the temperature and heat flux fields across the boundary. A CNT is modeled as an ellipsoidal inclusion, surrounded by an interphase (thermal barrier) material of ellipsoidal shape and an infinitely extended matrix phase beyond that. A set of permissible functions that satisfy the homogeneous boundary condition and the heat-flux/temperature continuity conditions across each interface are derived. The temperature field in the CNT composite is expressed by a linear combination of the permissible functions. The effects of the interphase properties as well as the geometrical shape of CNTs on the heat conduction are assessed.

2 Formulations

The energy equation fot the temperature field, u, under steady-state heat conduction is expressed as

$$Lu = 0, \tag{1}$$

where L is a differential operator defined as

$$Lf \equiv \nabla \cdot \left(K \left(\nabla f \right) \right). \tag{2}$$

The quantity, K, is the thermal conductivity, $\nabla \cdot$ is the divergence operator and ∇ is the gradient operator. Equation (1) along with the prescribed boundary condition constitutes a boundary value problem.

A CNT is modeled as an ellipsoidal inclusion coated by a thermal barrier of ellipsoidal shape in an infinitely extended matrix phase. Each ellipsoid is expressed by

$$\left(\frac{x}{a_i}\right)^2 + \left(\frac{y}{b_i}\right)^2 + \left(\frac{z}{c_i}\right)^2 \le 1, \tag{3}$$

where a_i, b_i and c_i are the lengths of the axis for each ellipsoid.

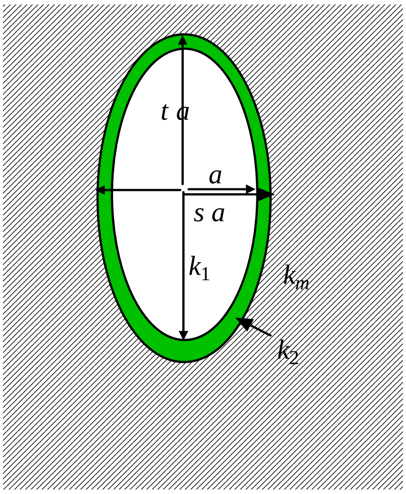

Fig. 1. Three-phase model

In order to obtain the temperature field in such a medium, a set of admissible functions for each phase is introduced as

$$f_1(x,y,z) = \sum_{i,j,k} a_{ijk} x^i y^j z^k, \tag{4}$$

$$f_2(x,y,z) = \sum_{i,j,k} b_{ijk} x^i y^j z^k, \tag{5}$$

$$f_m(x,y,z) = \sum_{i,j,k} c_{ijk} x^i y^j z^k e^{-(x/a)^2-(y/b)^2-(z/c)^2}, \tag{6}$$

where $f_1(x,y,z)$ is a polynomial function for the CNT phase, $f_2(x,y,z)$ is a polynomial function for the thermal barrier phase and $f_m(x,y,z)$ is a function for the matrix phase that vanishes at infinity. The indices, 1, 2 and m, refer to the CNT phase, the thermal barrier phase and the matrix phase, respectively.

The unknown coefficients, a_{ijk}, b_{ijk} and c_{ijk} are determined in such a way that they satisfy the following continuity conditions at each interface:

$$f_1 = f_2, \tag{7}$$

$$k_1 \frac{\partial f_1}{\partial n} = k_2 \frac{\partial f_2}{\partial n}, \tag{8}$$

$$f_2 = f_m, \tag{9}$$

$$k_2 \frac{\partial f_2}{\partial n} = k_m \frac{\partial f_m}{\partial n}. \tag{10}$$

Equations (7)-(8) are at the interface of the CNT and the thermal barrier and equations (9)-(10) are at the interface of the thermal barrier and the matrix. Using a computer algebra system, it is possible to obtain the explicit forms of f_1, f_2 and f_3 with all the parameters present.

When the CNT composite is subject to uniform heat flux at infinity (far field), the unknown temperature field, u, can be expressed as

$$u = \mathbf{X}\cdot\mathbf{x} + \sum_{\alpha}^{N} c^\alpha f^\alpha(x), \tag{11}$$

where f^α is an α-th admissible function defined for each phase (consisting of three different functions, f_1^α, f_2^α and f_m^α) and $\mathbf{X}$ is a constant temperature gradient at infinity defined as

$$\mathbf{X} \equiv \nabla u \quad x \to \infty. \tag{12}$$

From equation (11),

$$\nabla u = \mathbf{X} + \sum c^\alpha \nabla f^\alpha. \tag{13}$$

By taking the average over the entire composite,

$$\frac{1}{V}\int_V \nabla u dV = \mathbf{X} + \sum c^\alpha \frac{1}{V}\int_V \nabla f^\alpha dV, \tag{14}$$

so for the average of ∇u to be equal to $\mathbf{X}$, the following has to be satisfied

$$\lim_{V\to\infty} \frac{1}{V}\int_V \nabla f^\alpha dV = 0, \tag{15}$$

This is automatically satisfied as f^α is chosen to vanish as $x \to \infty$.

Now apply L on the both sides of equation (10) to get

$$\begin{aligned} Lu &= L(\mathbf{X}\cdot\mathbf{x}) + \sum c^\alpha L f^\alpha \\ &= 0 \end{aligned} \tag{16}$$

or

$$\sum c^\alpha L f^\alpha = -L(\mathbf{X}\cdot\mathbf{x}). \tag{17}$$

Multiply f^β on the both sides of the above to get

$$\sum c^\alpha \left(Lf^\alpha, f^\beta\right) = -\left(L(\mathbf{X}\cdot\mathbf{x}), f^\beta\right), \tag{18}$$

where (f,g) is defined as

$$(f,g) \equiv \int_V f(x)g(x)dV. \tag{19}$$

By defining

$$a_{\alpha\beta} \equiv \left(Lf^\alpha, f^\beta\right), \quad b_\alpha \equiv -\left(L(\mathbf{X}\cdot\mathbf{x}), f^\alpha\right). \tag{20}$$

Equation (16) is converted to an algebraic equation as

$$A\mathbf{c} = \mathbf{b}, \tag{21}$$

where

$$\begin{aligned} a_{\alpha\beta} &= (Lf^{\alpha}, f^{\beta}) \\ &= \int_V \nabla\cdot\left(K\nabla f^{\alpha}\right) f^{\beta} dV \\ &= -\int_V K\nabla f^{\alpha}\cdot\nabla f^{\beta} dV \\ &= -\sum_{i=1}^{3} K^i \int_{\Omega_i} \nabla f_i^{\alpha}\cdot\nabla f_i^{\beta} d\Omega_i . \end{aligned} \tag{22}$$

and

$$\begin{aligned} b_{\alpha} &= -\left(L(\mathbf{X}\cdot\mathbf{x}), f^{\alpha}\right) \\ &= -\int_V \nabla\cdot\left(K\nabla\left(\mathbf{X}\cdot\mathbf{x}\right)\right) f^{\alpha} dV \\ &= \mathbf{X}\cdot\int_V K\nabla f^{\alpha} dV \\ &= \mathbf{X}\cdot\sum_{i=1}^{3} K^i \int_{\Omega_i} \nabla f_i^{\alpha} d\Omega_i , \end{aligned} \tag{23}$$

where the fact that f_m vanishes at infinity was used. Therefore, by solving a set of algebraic equations, (21), the temperature field can be expressed by equation (11).

The effective thermal conductivity, k^*, of general heterogeneous materials is expressed as

$$k^* = k^m + \sum_{i=1}^{N} v_i (k^i - k^m) A_i , \tag{24}$$

where k^m is the matrix thermal conductivity, k^i is the thermal conductivity for the i-th phase, v_i is the volume fraction for the i-th phase and A_i is the temperature gradient proportionality factor defined as

$$\nabla u \,(\text{in the i}-\text{th phase}) = A_i < \nabla u >, \tag{25}$$

where ∇u is the temperature gradient in the i-th phase and $< . >$ denotes the volume averaged quantity. Equation (24) implies that if the temperature gradient field inside a CNT is known, the effective thermal conductivity can be computed using equation (24).

3 Example

The expressions for permissible functions are too lengthy to be included in this paper. The following are examples of permissible functions for a 2-D elliptical shaped CNT/barrier embedded in the 2-D matrix phase extended to infinity:

$$\begin{cases} f_1^{\alpha} = -\dfrac{k_2 s^4 t^2 a^4}{k_m} - \dfrac{1}{2} s^4 t^2 a^4 - \dfrac{k_2 t^2 a^4}{k_1} + \dfrac{t^2 a^4}{2} + \dfrac{k_2 t^2 x^2 a^2}{k_1} + \dfrac{k_2 y^2 a^2}{k_1} \\ f_2^{\alpha} = \dfrac{t^2 x^4}{2} + y^2 x^2 + \dfrac{y^4}{2t^2} - \dfrac{2a^4 k_2 t^2 s^4 + a^4 k_m t^2 s^4}{2k_m} \\ f_m^{\alpha} = -\dfrac{a^4 e^{-\frac{x^2}{a^2 s^2} - \frac{y^2}{a^2 s^2 t^2} + 1} k_2 s^4 t^2}{k_m} , \end{cases} \tag{26}$$

$$\begin{cases} f_1^{\beta} = a^2 t^2 - a^2 s^2 t^2 - \dfrac{a^2 k_2 s^2 t^2}{k_m} + \dfrac{k_2 x^2 t^2}{k_1} - \dfrac{a^2 k_2 t^2}{k_1} + \dfrac{k_2 y^2}{k_1} \\ f_2^{\beta} = t^2 x^2 + y^2 - \dfrac{a^2 k_2 s^2 t^2 + a^2 k_m s^2 t^2}{k_m} \\ f_m^{\beta} = -\dfrac{a^2 e^{-\frac{x^2}{a^2 s^2} - \frac{y^2}{a^2 s^2 t^2} + 1} k_2 s^2 t^2}{k_m} \end{cases} \tag{27}$$

where t is the aspect ratio of the ellipses, a is the minor axis of the first ellipse and sa is the minor axis of the surrounding ellipse

The obtained permissible functions are used in equations (22) and (23) to compute the elements of $a_{\alpha\beta}$ and b_{α}. The following integral formulas were used.

$$\iint x^m y^n dxdy = \frac{a^{m+1} b^{n+1}}{4} \frac{\Gamma\left(\frac{m+1}{2}\right)\Gamma\left(\frac{n+1}{2}\right)}{\Gamma\left(\frac{m+n}{2}+1\right)} \frac{2}{2+m+n}, \tag{28}$$

where

$$0 \le \left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 \le 1. \tag{29}$$

$$\iint x^m y^n e^{-\left(\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2\right)} dxdy = \frac{a^{m+1} b^{n+1}}{4} \frac{\Gamma\left(\frac{m+1}{2}\right)\Gamma\left(\frac{n+1}{2}\right)}{\Gamma\left(\frac{m+n}{2}+1\right)} \Gamma\left(\frac{2+m+n}{2}, 1\right), \tag{30}$$

where

$$1 \le \left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 \le \infty, \tag{31}$$

and $\Gamma(n,1)$ is the incomplete Gamma function.

Figure 2 shows the temperature distribution inside the CNT, The thermal conductivity for the CNT, the thermal barrier and the matrix are chosen as 3,000 W/mk, 12 W/mk and 0.2 w/mk, respectively [3]. The aspect ratio of the CNT is chosen as 300.

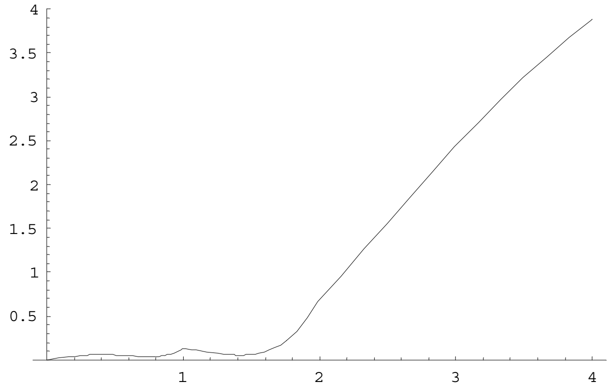

Fig. 2. Temperature distribution around CNT

It is found that the temperature field is not influenced by the aspect ratio of the CNT as long as the ratio is over 100. With the difference of thermal conductivities between the CNT and the matrix over 6,000 times, the temperature inside the CNT is almost flat and variation of the temperature is seen in the thermal barrier phase.

4 Conclusions

The temperature field of carbon nanotube composites with a thermal barrier was derived with the permissible functions that satisfy the interface continuity conditions exactly. The effective thermal conductivity of such a composite can be evaluated using the approach in this paper. Although the CNT was modeled as an ellipsoid surrounded by another ellipsoidal coating barrier, a tubular shape is close to the real CNT composite.

References

[1] Thostenson E. T., and Chou T-W., "On the elastic properties of carbon nanotube-based composites: modelling and characterization," *J. Phy. D: App. Phy.*, 36(5): pp.573-582, 2003.

[2] Bagchi, A. and Nomura, S., "On the effective thermal conductivity of carbon nanotube reinforced polymer composites," *Composites Science and Technology*, vol. 66, pp.1703-1712, 2006.

[3] Nan, C-W., Liu, G., Lin, Y. and Li, M., "Interface effect on thermal conductivity of carbon nanotube composites," *J. App. Phys. Lett.*, 85, pp.3549-3551, 2004.