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Evaluation of effective thermal conductivity for carbon nanotube/polymer composites using control volume finite element method

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Abstract

Effective thermal conductivity of the polymeric composites filled with carbon nanotubes (CNTs) is predicted by using the asymptotic expansion homogenization technique (AEH), which makes it possible to localize and homogenize a heterogeneous medium. In the present study, CNT embedded epoxy composites are taken into account as the heterogeneous system. The representative volume element (RVE) employed in the homogenization process is constructed by assuming that the CNTs are dispersed homogeneously in the polymer matrix. It is presumed that the RVE contains a single CNT and that there is no direct interaction between neighboring CNTs. The dispersion state of CNTs in the composites is morphologically characterized by the field emission scanning electronic microscope (FESEM). In order to consider the orientation state of CNTs, the bounding approach is adopted by using the orientation tensor. It is found that the numerically homogenized thermal conductivity is higher than that obtained by the analytic model. Predicted conductivities are also compared with experimental results as well as analytic results. The homogenization technique yields the effective thermal conductivity accordant with experimental results. In the case that a heterogeneous material has anisotropic properties or geometrical complexity, the homogenization technique is an efficient method to obtain averaged material properties equivalent to those of the real heterogeneous medium.

Keywords: Carbon nanotubes; Resins; Thermal conductivity

1. Introduction

Carbon nanotubes (CNTs) have been extensively studied due to their outstanding physical properties such as high Young's modulus, electrical and thermal conductivities. The CNT is of keen interest to scientists and engineers, because it has many potential applications including nanoprobes, field electron emitter, hydrogen absorber, nanotweezer, nanobearing, and so on [1]. In order to achieve the superior properties, polymeric composites filled with the CNTs have been investigated vigorously for a few years [2–4]. Recent studies show that the CNT embedded composite has excellent conductive properties and is one of promising materials which can be used for production of miniature devices managing heat transfer. Some experiments have been carried out to measure thermal conductivities of the single walled carbon nanotube (SWNT) and the multiwalled carbon nanotube (MWNT) [5–7]. However, the measured thermal conductivity varied drastically from 30 to 3000 W/m K. Moreover, some of the thermal conductivities calculated based on the molecular dynamics (MD) simulation were as high as 6000 W/m K at room temperature for an isolated SWNT [8–10]. On the other hand, it is known that carbon fiber and carbon fiber reinforced carbon/carbon (CC) composites have thermal conductivities less than 600 W/m K [11]. Recently, quite a

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few studies on thermal conductivity of CNT-based composites are reported but most of them are conducted experimentally or analytically [12–14] and there are few reports associated with numerical calculation of the thermal conductivity [15,16]. Since the MD simulations are restricted to small length and time scales, they cannot directly handle the CNT/polymer composites with the present computing capabilities.

In conventional composites filled with fibers and particles, the homogenization technique using a representative volume element (RVE) has been employed in the past few years to obtain effective thermal conductivity of the composites numerically [17–27]. Taghite et al. [17] examined a thermal problem with the Fourier boundary conditions at each edge of holes in a heat exchanger consisting of periodically perforated plates and estimated temperature field in the upper plate by using a homogenization technique. Chung and Tamma [18] computed a nonlinear thermal heat conduction problem with temperature dependent conductivity by applying the asymptotic expansion homogenization (AEH) approach. It was shown that the AEH approach for homogenizing nonlinear properties of composite materials was renowned due to its ability to deal with complex microstructural shapes. Rocha and Cruz [19] calculated effective thermal conductivity of unidirectional fibrous composite materials with interfacial thermal resistance between the continuous and dispersed phases. They showed that the linear finite element method is not appropriate for composites with large ratio of conductivities between two phases. Mongi and Hassan [20] solved a homogenization problem for a heterogeneous medium composed of three components. The asymptotic behavior of global temperature field in the three phases was represented. Kamiński [21,22] performed the homogenization of transient heat transfer problem, where mathematical model was used based on the effective modules implemented by a finite element method. He calculated the effective thermal conductivity in the closed form. Asakuma et al. [23] analyzed the effective thermal conductivity of a metal hybrid bed using a homogenization method.

In this study, the effective thermal conductivity tensor of CNT filled composites was examined by using a homogenization method. The effects of the aspect ratio and the concentration of CNTs on the thermal conductivity are investigated. In contrast to most of the previous studies on the homogenization method using the FEM, control volume finite element (CVFEM) is adopted in the implementation of the homogenization method. In order to compare the numerical results with analytic ones, the analytic model proposed by Lewis and Niesen [28] is employed. The predicted thermal conductivities are also verified through comparison with experimental results.

2. Homogenization approach

Homogenization method is a powerful tool by which a heterogeneous medium is transformed to the equivalent homogeneous medium with the same internal energy. The asymptotic expansion homogenization (AEH) method adopted in this study is able to perform both localization and homogenization for the heterogeneous medium. In multiscale approach, the homogenization and the localization are the main concerns: the former yields smeared material properties used in the macroscopic field equations and the latter provides estimation of the microscopic material behavior based on the macroscopic solution. In order to implement the homogenization technique, the representative volume element (RVE) for real composites with periodic structure and scale parameter relating dimensions of the RVE to those of the entire composite are employed. The scale parameter must approach zero or very small positive value.

2.1. Formulation

Several assumptions are made for theoretical modeling. Firstly, CNTs are homogeneously dispersed in the CNT/polymer composites and have uniform dimensions including their length, inner, and outer diameters. Secondly, there is no direct interaction between the adjacent CNTs. Lastly, the CNT composites contain the periodic unit cell which includes a single CNT embedded unidirectionally as shown in Fig. 1. The orientation effect of CNTs will be taken into account in later section. The periodic unit cell consists of three different regions, i.e., matrix, CNT, and air which are denoted by Ω_m, Ω_c, and Ω_a, respectively. Each region has its own thermal conductivity. Fig. 1(b) shows the RVE constructed by assuming square packing of the CNTs. The scale parameter, ε, which is the ratio of characteristic length scales, is given by the following equation:

$$\varepsilon = \frac{l}{L} \ll 1 \tag{1}$$

The equation means that the entire dimension, Ω, of RVE is small enough to be neglected compared with the characteristic length, L, for the entire composites.

In steady-state heat conduction problem, the governing equation for each region is expressed as below:

$$-\frac{\partial}{\partial x_i}\left(k_{ij}^{\mathrm{m}}\frac{\partial T}{\partial x_j}\right) = f_{\mathrm{m}} \quad \text{in } \Omega_{\mathrm{m}} \tag{2}$$

$$-\frac{\partial}{\partial x_i}\left(k_{ij}^{\mathrm{c}}\frac{\partial T}{\partial x_j}\right) = f_{\mathrm{c}} \quad \text{in } \Omega_{\mathrm{c}} \tag{3}$$

$$-\frac{\partial}{\partial x_i}\left(k_{ij}^{\mathrm{a}}\frac{\partial T}{\partial x_j}\right) = f_a \quad \text{in } \Omega_{\mathrm{a}} \tag{4}$$

where k_{ij}^{m}, k_{ij}^{c}, and k_{ij}^{a} are the second order thermal conductivity tensors for matrix, CNT, and air, respectively. f_{m}, f_{c}, and f_{a} denote the volumetric heat generation for each region. In this study, the heat generation is not considered and the thermal conductivity tensor is assumed to be independent of temperature. The temperature field is asymptotically expanded as below: