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Effects of thermal contact resistance on the thermal conductivity of core–shell nanoparticle polymer composites

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ABSTRACT

This paper describes a numerical study on the thermal conductivity (TC) of core–shell nanoparticle polymer composites under the effects of thermal contact resistance (TCR), in addition to other parameters. Finite element method is used for both numerical simulation and solving the related nonlinear equations. Consequently, the effective thermal conductivity (ETC) depends significantly on the TCR, and it decreases sharply for larger volume fractions (VF) and larger TC of core–shell. The ETC from the present study matches well with that obtained by Felske model only if the TCR is negligible. Core VF of 0.516 times greater than that of shell is a necessary condition for an existence of the maximum ETC regardless of the presence of the TCR. In addition, the ETC is independent on the TCR at core–shell interface when either the TCR at shell-matrix interface is large or the TC of shell approaches a critical value. Many other good guidance are provided for enhancing the TC of core–shell nanoparticle polymer composites, and it plays an important role in producing advanced polymer composites.

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1. Introduction

Enhancing the thermal conductivity (TC, hereafter) of polymers by adding organic or inorganic micro-/nanoparticles with higher TC is becoming increasingly important in producing advanced polymer composites. Potential applications of such composites include electronic packaging and encapsulations, satellite devices, and areas where good heat dissipation, low thermal expansion, and light weight are required [1,2]. The TC of polymers is known to be commonly very low, and it has traditionally been enhanced by adding fillers (dispersed phase) such as graphite, carbon black, carbon fibers, and ceramic or metal particles with high TC, into matrix materials (continuous phase). It is evident that polymer composites containing highly conductive fillers have advantages due to their easy processability, low cost, and durability against corrosion. More reasons for the use of fillers can be found in [3].

In order to predict the TC of particle-filled composite materials, a variety of theoretical and empirical models have been provided for a number of years [4]. For example, Maxwell model [5], Lewis and Nielsen model [6,7], Agari and Uno model [8], or Bruggeman model [9] are some well-known models which have been widely used in literature. However, each TC model shows to be valid for only one or some of composites, and it depends on the characteristic quantities, for example the volume fraction (VF) of filler, the TC ratio between filler and the matrix, the filler shape and orientation. Tavman [10] indicated that the Agari and Uno model effectively estimates the TC of aluminum powder-filled high-density polyethylene composites at high filler content. He et al. [11] reported that both the effective medium theory (EMT) and Nielsen models can predict well the TC at a low filler VF. Most of these models were considered to predict the TC of composites containing a single filler (also called mono-particle filler) [12], thus other types of filler should be considered extensively for enhancing the TC of polymers.

Indeed, the TC of polymers can be enhanced using various types of filler such as mono-particle filler, two or more components in combination. For example, single fillers are being used, and the TC of such polymer composites can be predicted using theoretical and empirical models mentioned above. The synergic effect of hybrid filler (two particles with the same or different properties and sizes) in improving the TC was also investigated in [13–16]. Furthermore, Gao and Zhao [17] considered the effects of nanofillers on the TC of epoxy, and suggesting that the TC can be effectively improved using different fillers, single fillers, hybrid fillers, and particularly the combination of three fillers. The TC of composite was shown to not only depend on filler properties, but it also depends on other effects like the formation of conductive chains and heat transfer networks.

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Recently, a new type of filler, core–shell nanoparticle has been regarded as a promising candidate for enhancing the TC of polymer composites. Zhou et al. [18] indicated that the TC was remarkably improved by adding core–shell Ag/SiO2 nanoparticles into polyimide matrix. Kim et al. [19] reported the significant enhancement of the TC using FeCr metal core–aluminum oxide shell particles with a highly mesoporous shell layer compared to the use of uni-modal particles. In addition, Thiele et al. [20] investigated numerically and discussed about some effects of specific parameters, the VF and TC of core and shell on the TC of composites containing spherical core–shell capsules. More recently, Ngo and Byon [21] have performed an extensive study on the TC of core–shell nanoparticle polymer composites, and provided optimum conditions for enhancing and achieving the maximum TC. While these studies have examined the effectiveness of core–shell particles to the TC, very limited number of them considers the effects of thermal contact resistance (TCR) on the TC of such polymer composites. These effects were demonstrated to play an importance role in the TC enhancement of advanced polymer composites used in potential applications [22–25].

The purpose of this study is to describe and examine the effective thermal conductivity (ETC) of core–shell nanoparticle polymer composites under the effects of the TCR, in addition to other parameters, the TC ratios between spherical core nanoparticles, shell layer and the matrix material, and the VFs of core and shell. A numerical method is used for both simulating the thermal flow through such composite structure and solving a nonlinear Ordinary Differential Equation (ODE) originated from Felske model. The thermal behaviors of core–shell nanoparticle polymer composites under the effects of TCR at shell-matrix and core–shell interfaces are discussed in detail.

2. Numerical method

2.1. Mathematical formula

Fig. 1 shows a numerical model as well as boundary conditions. In this figure, a unit cell can be utilized as a control volume since the number of spherical-core–shell nanoparticles dispersed throughout the matrix material is very large. It is assumed that

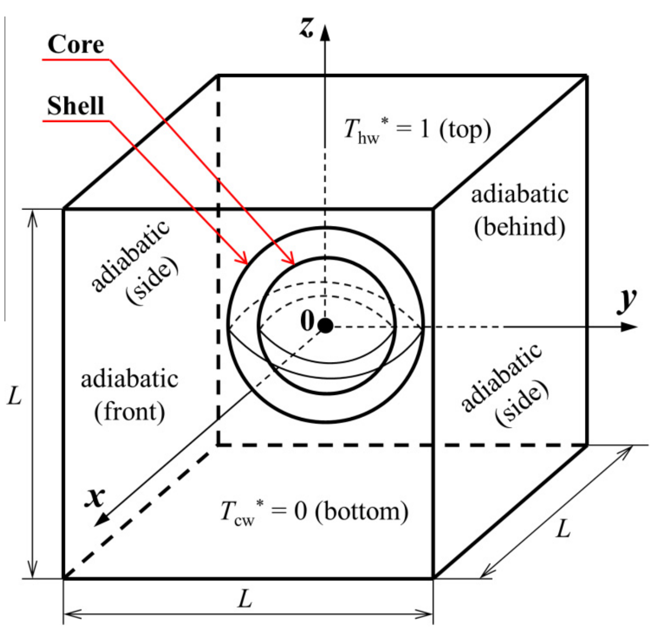

Fig. 1. Numerical model and boundary conditions.

the nanoparticles are isolated, thus total VF of core–shell considered is less than about 0.52 and 0.74 for single core–shell and face-centered cubic (FCC) arrangement shown in Fig. 2, respectively. In addition, the TCs are assumed to be constant for all core nanoparticles (k_c), shell layer (k_s), and the matrix materials (k_m).

The thermal flow through a composite structure is considered to be homogeneous with no heat source. Laplace equations can be therefore used to describe the heat transfer, which are given by

$$\frac{\partial}{\partial x}\left(\frac{\partial T_i}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{\partial T_i}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{\partial T_i}{\partial z}\right)=0 \quad i=c,s,m \tag{1}$$

The subscripts "c", "s" and "m" denote for the spherical-core nanoparticle, shell layer and matrix material, respectively. The following non-dimensional variables are introduced:

$$x^*=\frac{x}{L};\quad y^*=\frac{y}{L};\quad z^*=\frac{z}{L};\quad T_i^*=\frac{T_i-T_{cw}}{T_{hw}-T_{cw}} \tag{2}$$

where the characteristic length in this problem is L, the dimension of a unit cell, as shown in Fig. 1. Consequently, Eq. (1) can be rewritten in non-dimensional form as:

$$\frac{\partial}{\partial x^*}\left(\frac{\partial T_i^*}{\partial x^*}\right)+\frac{\partial}{\partial y^*}\left(\frac{\partial T_i^*}{\partial y^*}\right)+\frac{\partial}{\partial z^*}\left(\frac{\partial T_i^*}{\partial z^*}\right)=0 \quad i=c,s,m \tag{3}$$

The boundary conditions are also shown in Fig. 1. All side walls are considered as adiabatic walls, and isothermal conditions are applied at the top and bottom walls. As a result, the temperature difference between the inlet (top) and outlet (bottom) is controllable and the thermal flow mainly moves along z direction. The effect of the TCR is considered extensively in the present study. The contact interface between the particles and the matrix is modeled as a thin-virtual shell with uniform thickness d_{int} and TC k_{int} [22]. In simulation, the following boundary conditions are imposed at the interface between two different materials:

$$\begin{cases} -n_a.\nabla T_a^* = -\frac{T_b^*-T_a^*}{R_c^*} \\ -n_b.(\kappa\nabla T_b^*) = -\frac{T_a^*-T_b^*}{R_c^*} \end{cases} \tag{4}$$

In Eq. (4) above, the TCR (R_c) is defined in a non-dimensional form:

$$R_c^* = R_c\frac{k_m}{L} = \frac{d_{int}^*}{k_{int}^*} \tag{5}$$

where k_{int} is considered as the harmonic mean TCs of two materials. According to this definition, the TC of the interface is slightly higher than that of a material with lower TC, which is in good agreement with the assumptions by Tsekmes et al. [26]. In addition, the interface thickness is normalized by the characteristic length of the unit cell. Consequently, the non-dimensional forms of d_{int} and k_{int} shown in Eq. (5) are represented by Eq. (6). Notably, there are two

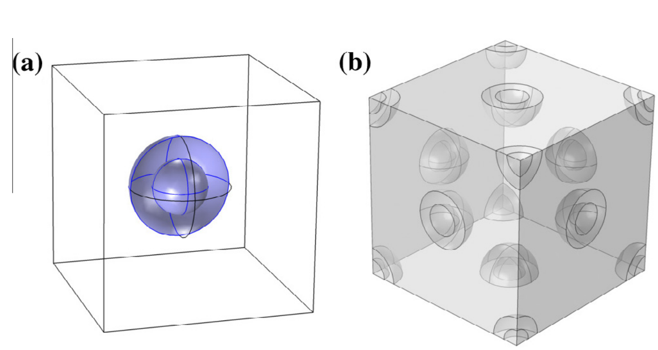

Fig. 2. Unit cells used for simulation. (a) Single core–shell filler, and (b) Face-centered cubic (FCC) arrangement of core–shell filler.

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