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A Numerical Analysis for Predicting the Thermal Conductivity of Carbon Nanotube Reinforced Copper-Matrix Nanocomposites

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Abstract. Thermal conductivity of carbon nanotubes (CNTs) copper-matrix nanocomposites was predicted by using numerical approach. In the present study, twenty representative volume elements (RVEs) were modeled by assuming that the CNTs are distributed homogeneously in the copper (Cu) matrix. It is assumed that each RVE contains different pattern of CNTs distribution while the direction, diameter and length of CNTs are held constant. The effect of the CNTs-matrix interfacial resistance was also negligible. Therefore, it was observed that the predicted values of thermal conductivity would reach to the upper-bound rule of mixtures.

1 Introduction

Having a Young's modulus of more than 1 TPa, estimated tensile strength of over 150 GPa, and thermal conductivity K up to 6000 W/mK [1-4], CNTs are ideal reinforcement for advanced composites materials for various engineering applications such as aerospace, energy, oil and gas, medicine, automotive, and electronic devices. Over the last decade, numerous works have focused on the enhancement of the thermal conductivity for polymer matrix composites. While only limited work were conducted for metal matrix composites. Recently, due to the high thermal and electrical conductivity of Cu and its potential applications for various electronic devices, the interest in using Cu as a matrix in nanocomposite materials has increased. However, due to some difficulties such as achieving homogenous dispersion of CNTs within metal matrices especially at high CNTs loading and lack of suitable synthesis techniques [5, 6], research on metal-matrix composites has been to some extent limited. Maintaining a homogeneous distribution of CNTs in the matrix, loss of CNTs during processing, interfacial reactions and bonding with the matrix are some of the critical issues which have been the main concerns among scientists in the fabrication of CNTs metal-matrix nanocomposites [7, 8]. To overcome these challenges, different fabrication processes such as thermal spraying [9], hot pressing [10], hot extrusion [11] and spark plasma sintering (SPS) [12] have been proposed by researchers.

In spite of recent progress in improving the dispersion of CNTs in Cu matrix, the remarkable amount of agglomeration of CNTs at the Cu grain boundaries have also been reported [13, 14]. This

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defect has a direct impact on the properties of such nanocomposites which results in lower thermal conductivity than expected. A novel processing technique has recently been proposed by Chu et al. [15] to fabricate CNT/Cu nanocomposites. It used the particles-compositing method to distribute CNTs uniformly in the Cu matrix. Using this technique, the agglomerated CNT ropes or lumps have been disintegrated into the individual CNTs. Although a good dispersion was reported, the enhancement in the thermal conductivity of fabricated CNTs/Cu composites was not measured.

Kim et al. [16] investigated the thermal conductivity of CNTs reinforced Cu matrix nanocomposites synthesized via the molecular-level mixing process followed by SPS. They found that the thermal conductivity of CNTs/Cu nanocomposites are lower than that of unreinforced Cu and is decreased by increasing the CNT volume fraction. The interfacial resistance between CNT and Cu has been reported as a reason of this property deterioration. The better enhancement in the value of K was reported by Cho et al. [17]. They studied the thermal conductivity of CNTs/Cu nanocomposites fabricated by using hetero-aggregation method based on a wet mixing process followed by SPS. They reported higher thermal conductivities for CNT/Cu nanocomposites than that of unreinforced Cu up to 3% CNT volume fraction. However, a descending trend was reported for the values of K after reaching a pike of 359.2 W/m.K for the 1% CNT volume fraction. The thermal conductivity values even lower than that of unreinforced Cu were also reported for about 5% and 10% of CNT volume fractions.

Several factors were reported as the cause of the loss in the overall thermal conductivity of the composites such as interface thermal resistance, porosities, inhomogeneous distribution and incomplete consolidation [10-14]. As it has been mentioned in the literature, the thermal conductivity of composites materials are highly influenced by the distribution factor. That is to say, the more uniform and homogeneous CNTs dispersion are, the higher thermal properties would be achieved. Besides, CNT has ultra-high conductivity along the tube direction. Therefore, the thermal conductivity of the composites could be greatly improved when reinforced by the unidirectional CNT fibers. The purpose of this research is to predict the thermal conductivity of CNT/Cu nanocomposites using numerical analysis which has never been reported in the literature to the best knowledge of the author. For this purpose, several models of Cu-matrices reinforced with CNT fibers have been simulated based on the following assumptions:

- CNT fibers were being distributed homogeneously and unidirectionally in which all tubes were arranged along a heat transfer direction.
- The fiber-matrix interface thermal resistance is negligible.

2 Finite-Element Numerical Approach

In the present study, the same as in our previous work [18], 3-dimensional (3D) finite element modelling was carried out using the commercial MSC.Marc software to evaluate thermal conductivity of CNT/Cu nanocomposites. The representative volume elements (RVEs) considered for this study is shown in Fig 1. The RVE has a dimension of 60×60×300 nm3 filled with copper as the matrix material having sintered thermal conductivity of 330 W/m.K. Subsequently, the RVE was meshed and divided into the smaller elements and nodes which were used later as places for CNTs distribution. CNTs considered in this study have a length, diameter and thermal conductivity of 50 nm, 1.4 nm and 3000 W/m.K respectively. In total, twenty RVEs have been categorized into four different groups based on the CNT volume fractions with each of the distinct group having a peculiar CNT arrangement. The kind of CNTs arrangement was determined by the number of nodes in the RVE. This meant that the number of possible places that could be occupied by CNTs increase as the number of nodes in the RVE increased. A Matlab program has been developed to create the random distribution of CNTs inside the RVE.

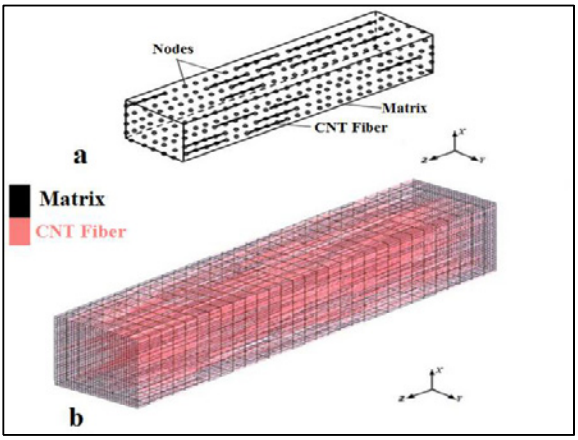

Fig. 1. a. Schematic representation of the RVE model. b. Nanocomposite model containing 2000 unidirectional CNT fibers (volume fraction = 10%).

In the evaluation of thermal conductivity, a temperature difference ΔT of 10°C was applied to the RVEs along the Z direction to obtain the heat flux q. The thermal conductivity of CNT reinforced composites K was then calculated using Fourier's law Eq. 1.

$$q = k\frac{\Delta T}{\Delta X} \quad (1)$$

3 Results and Discussion

The predicted thermal conductivity of CNT/Cu nanocomposites is given in Table 1. As shown in Table 1, different values of thermal conductivity were obtained for every constant CNT volume fraction. That is to say that thermal conductivity of nanocomposites is highly influenced by the variety of types of CNTs' distribution (arrangement) inside the matrix even when the orientations and the volume fractions of the CNTs are considered constant. This proves that there is an influence of the distribution of CNTs on the thermal conductivity of nanocomposites. These data also platted in Fig. 2 with comparison to Rule of Mixture and previous work by Chu et al. [15].

Table 1. Thermal conductivities of RVEs for various volume fractions.

Arrangement		CNT Volume Fraction [%]				
		0	2	5	7.5	10
Thermal Conductivity [W/m·K]	1	330	380.8	452.2	516.99	575.1
	2	330	379.8	451.3	515.28	571.2
	3	330	379.1	449.9	507.55	561.3
	4	330	375.9	440.2	505.7	561.3
	5	330	369.7	427.8	461.71	505.4

It is shown in Fig. 2 that the thermal conductivity of CNT/Cu nanocomposites increases with increasing CNT volume fraction. It is clearly seen that our predicted values without considering the effects of interface thermal resistance and agglomeration of CNTs yielded higher values of K than that of the experimental data. However, it could be deduced that the underperformance of the experimental values can be related to the unfavourable factors such as interfacial resistance between the Cu matrix and CNT reinforcement, porosity and inhomogeneous distribution of CNTs [15].

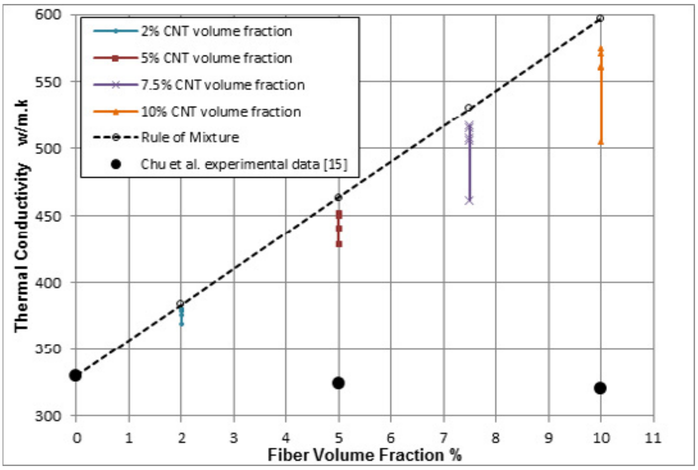

Fig. 2. Thermal conductivity of CNT/Cu nanocomposites versus CNT volume fraction.

4 Conclusion

In summary, 3D finite element models of CNT/Cu nanocomposites were developed and simulated using the commercial MSC. Marc software. Subsequently, the thermal conductivity of the nanocomposite models was predicted where enhancement in thermal conductivity compared to the unreinforced matrix was observed. It should be noted that the distribution of CNTs in the metal matrix played an important role in determining the thermal conductivity of nanocomposites, even when CNTs orientation and volume fraction were constant. Therefore, there were two requirements for achieving high thermal conductivity namely homogeneous dispersion of CNTs inside the matrix with less agglomeration and extremely low thermal resistance between CNTs and matrix. For that reason, more work needed to be done in the case of improving thermal properties of nanocomposites.

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