Determination of the thermal conductivity of Single wall Carbon Nanotubes Treated as Long Fiber for Reinforcing Aluminum Matrix composite

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ABSTRACT

Nanotechnology seeks to discover and manipulate the properties of matter at the nanoscale in order to develop new applications across many fields, such as electronics, and materials. These materials and systems can be designed to exhibit novel and significantly improved properties, phenomena, and processes as a result of the limited size of their constituent. Carbon nanotubes (CNTs) have stimulated enormous interest for conductive; energy storage and energy conversion devices; and nanometer-sized semiconductor devices.

In this paper, the thermal conductivity and density of CNT based Aluminum metal matrix are evaluated using a 3-D nanoscale representative volume element (RVE) using the finite element method software package. The results show that, with additions of the CNTs in a matrix at volume fractions of only about 3%, 7% and 11%, the density of the new composite reduced about 2% to 6%, and the thermal conductivity of the new composite varies linearly and increased by 9 to 10% with the change in volume fractions.

Keywords: Carbon nanotubes; Nanocomposites; Thermal conductivity; Finite element method; Aluminum

1. Introduction

The rising demand of higher performance but more compact electronic devices has created the need to make microprocessor chips faster and smaller. Heat dissipation becomes a thermal barrier to the performance of the chips. [1]

Aluminum is one of the most important engineering materials in many industrial applications. Aluminum has high electrical and thermal conductivities which made it more attractive in electronic packaging applications than aluminum. However, compared to the extensive works on aluminum-matrix composites, much less attention was paid on Aluminum-matrix composites. [2]

The invented material, the Carbon Nanotubes also has a high value of thermal conductivity. Carbon nanotubes (CNTs) are a promising reinforcement in composite materials to increase thermal conductivity, stiffness with low density because CNTs have very high thermal conductivity (> 3000 W/m.K) and low thermal expansion, excellent mechanical properties and relatively low density(1.3 to 1.8 g/cm^3) [3-5]. The developments of carbon nanotubes have rekindled the research in heat sink for next generation of microchip. These developments provide solution for rapid removal of heat from the electronic package. [6-7]

Until now, several attempts have been reported to fabricate CNT reinforced composite with various metallic (aluminum, copper, tungsten-copper, magnesium, etc.), ceramic (alumina, silicon carbide, magnesia) and polymeric (polyvinylidene fluoride, polyethylene, etc.) matrices [8-10].

However, Research on new materials technology is attracting the attention of researchers all over the world. Developments are being made to improve the properties of the materials and to find alternative precursors that can give desirable properties on the materials.
In this paper, 3D nanoscale square representative volume element is employed to investigate the thermal conductivity of carbon nanotubes treated as long fiber reinforced Aluminium metal matrix and the results are compared with some of theoretical models.

2. Materials and Methods

Representative Volume Element (RVE)

The representative volume element (RVE) plays a central role in the mechanics and physics of random heterogeneous materials with a view to predicting their effective properties and material microstructure[12]. The RVE used for analyzing long carbon nanotube reinforced iron matrix has a length, L = 10 nm. Carbon nanotube is embedded in the middle throughout the length of the composite as shown in Figure 1. The diameter of the carbon nanotube is varied according to the chiral indices Armchair, Zigzag, and Chiral ((5, 5), (5, 0), (5, 10)), respectively. The mean diameter (d_{mean}) of the CNT is obtained from this chiral index.[14, 15]

$$d_{mean} = \frac{\sqrt{3} * a_{c-c} \sqrt{(m^2)+(m*n)+(m^2)}}{\pi} \quad (1)$$

Where,
d_{mean} is the carbon nanotube mean diameter and,
a_{c-c} is the lattice distance between two carbon atoms
m, n are the carbon nano tube indices.

Assuming that thickness of the carbon nanotube is 0.34 nm
Assuming that the volume fraction used in this paper is 3, 7, and 11% respectively, the width (a) for the RVE can determined as follows:

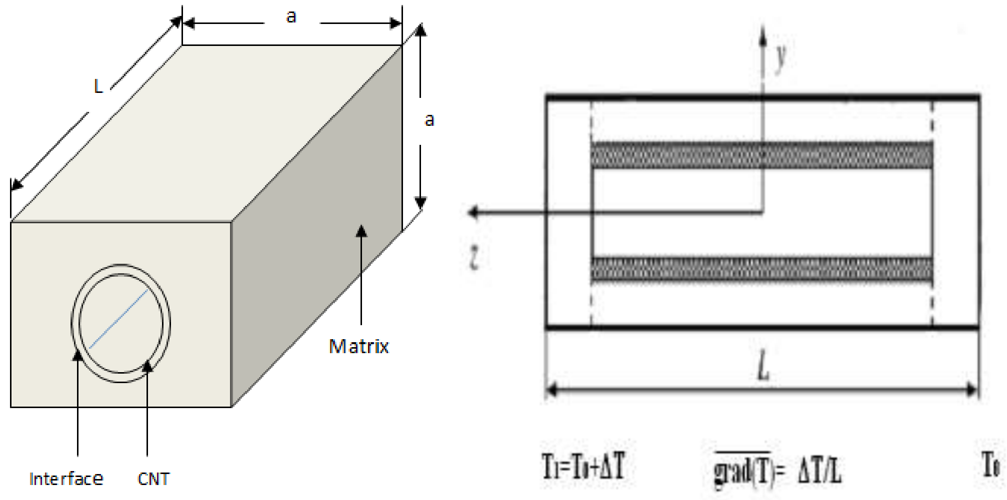


Figure 1: the representative volume element model and temperature imposed at boundary of the RVE

Table 1: ***The materials properties***

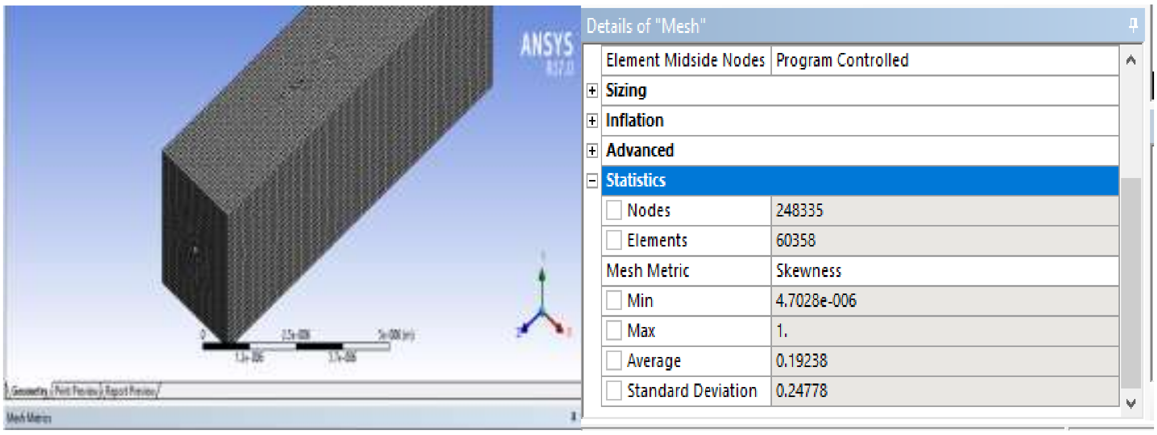
Property	**Matrix**	**Reinforcment**
	Aluminum (Al)	**Carbon Nanotube (CNT)**
Density (g/cm^3)	2.712	1.3
Thermal Conductivity (K) (W/m k) at 25°C	204	~3000

$$V_f = \frac{A_f L}{A_c L} \tag{2}$$

$$V_f = \frac{\pi(r_o^2 - r_i^2)}{a^2 - \pi r_i^2} \tag{3}$$

Where, V_f = Carbon nanotube volume fraction and a = Width of the square RVE
The material properties for the matrix and reinforcements and the schematic loading, elements and boundary condition of these models are shown in Figure 1 and Table 1.

In order to evaluate the effective thermal properties of composite, the finite element software package ANSYS is used. For simplification, there are many assumptions considered for the present analysis such as fibers are uniformly distributed in the matrix and perfectly aligned, and the interface between the fiber and matrix is perfectly bonded. The composite is free of voids and other irregularities. Finite element analysis may be desirable to simulate any case to predict the effective thermal properties. However, ANSYS model was developed for the numerical estimation of effective thermal conductivity using various RVEs. [16]
The representative volume element is divided into many regular volumes for meshing. First, all volumes of RVE are divided into equal eight parts, then, the representative volume element was divided into three parts of which the middle part corresponds to carbon nanotubes as shown in Figure 2. The representative volume element was meshed using hexahedron shaped element and mapped meshing algorithm. The longitudinal size is equal to the number of divisions in width is 10nm and number of divisions in thickness of carbon nanotube is three. Before meshing, different materials are assigned to the volumes for matrix and carbon nanotube. The element type used has eight nodes with a single degree of freedom, temperature, at each node. The element is applicable to a 3-D, steady-state or transient thermal analysis and can compensate for mass transport heat flow. [16, 17]



Details of "Mesh"

Element Midside Nodes	Program Controlled
⊞ Sizing	
⊞ Inflation	
⊞ Advanced	
⊟ Statistics	
☐ Nodes	248335
☐ Elements	60358
Mesh Metric	Skewness
☐ Min	4.7028e-006
☐ Max	1.
☐ Average	0.19238
☐ Standard Deviation	0.24778

Figure 2: Final RVE model and meshing

3. Results and Discussion

The theoretical estimation of the effective thermal conductivity of the carbon nanotubes reinforced composite was proposed, but that is not appropriate for the complex geometrical shape and arrangement of carbon nanotubes embedded in representative volume elements.

Prediction of the Nanocomposite Density:

As the volume fraction of the Carbon Nanotubes increase the density of the Carbon Nanotubes reinforced metal matrix Nanocomposite predicted to decrease linearly. Therefore, the higher the amount of Carbon Nanotubes used the lower density of the Nanocomposite is predicted to be. Figure 3 shows the density of the Carbon Nanotubes reinforced Aluminium matrixes Nanocomposite. It is found that the reduction in the density of the new Nanocomposite varied from 1% to 24% for Aluminum matrix when the volume fraction of the Carbon Nanotubes increased from 1% to 47%.

Effect of chiral index on the effective thermal conductivity of the Nanocomposite

The results for aluminium matrix reinforced by 3% volume fraction of different categories of carbon nanotubes are shown in Figure 4 and Table 2 show the temperature difference in Nanotubes and model. It can be noticed that the enhancement in thermal conductivity are varied from 9% to 10%. However, Figure 5 shows that as the volume fraction increases within tested range, the thermal conductivity increases linearly for all indexes but with different values. The zigzag index shows the highest value of thermal conductivity while the chiral index shows the lowest.

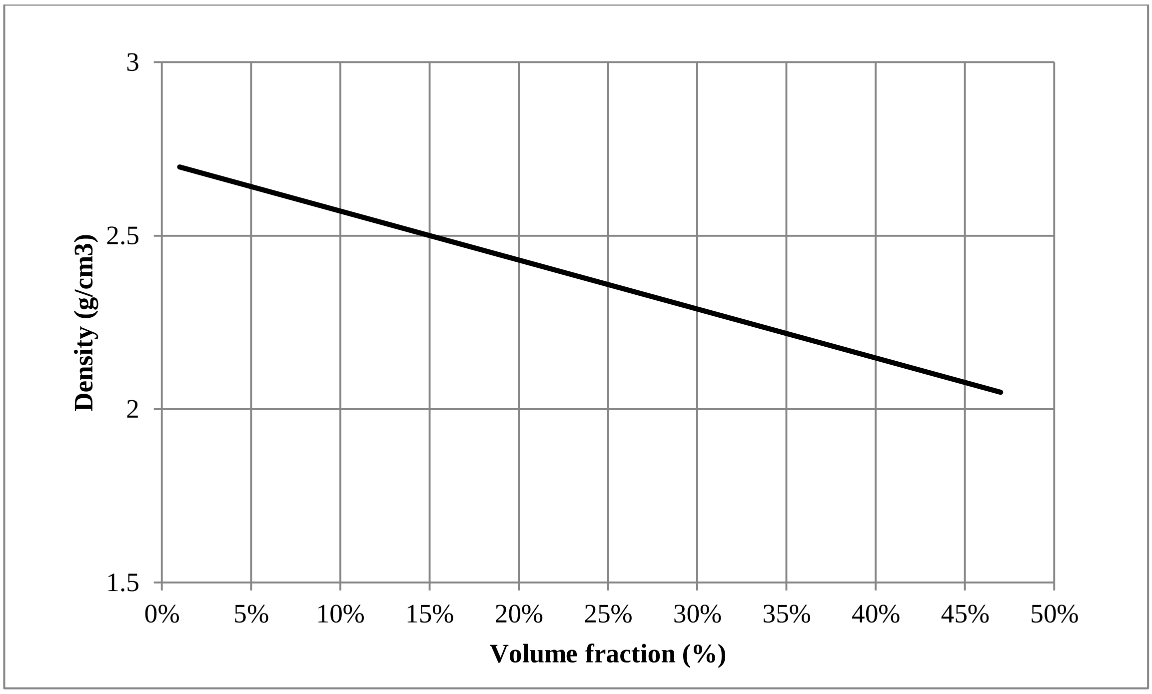


Figure3: Density of carbon nanotube reinforced Aluminum matrix

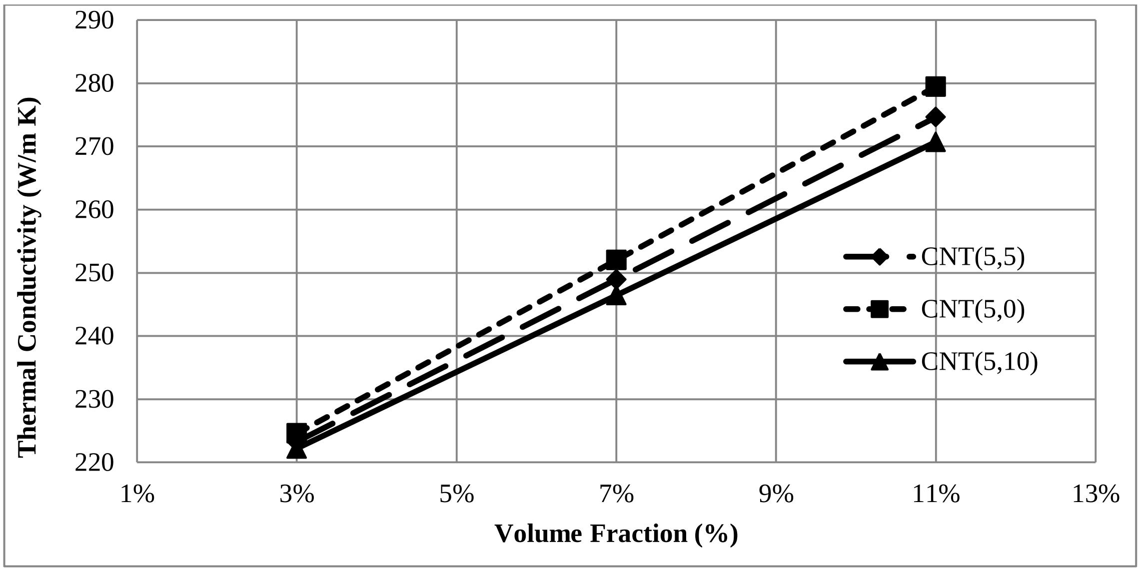


Figure 4: Effect of volume fraction on the thermal conductivity of different carbon nanotube chiral index reinforced aluminum metal matrix

Table 2**:** *Effect of chiral index of carbon nanotube reinforced Aluminium matrix on the thermal conductivity for different models (Vf=3%)*

Carbon Nanotube index	K (W/m K)	% change
(5,5)	223.269	9.4%
(5,0)	224.585	10.1%
(5,10)	222.196	8.9%

It can clearly appear that, the value of thermal conductivity for zigzag type is the highest, while for chiral type is the lowest.

It can be also observed that, as shown in Figures 5and 6 that the temperature distribution in the entire representative volume element is constant irrespective of Aluminium matrix material, but the magnitude of the thermal flux in z-direction depends on the Aluminium matrix material. In particular, distributions of the thermal fields are exactly equal.

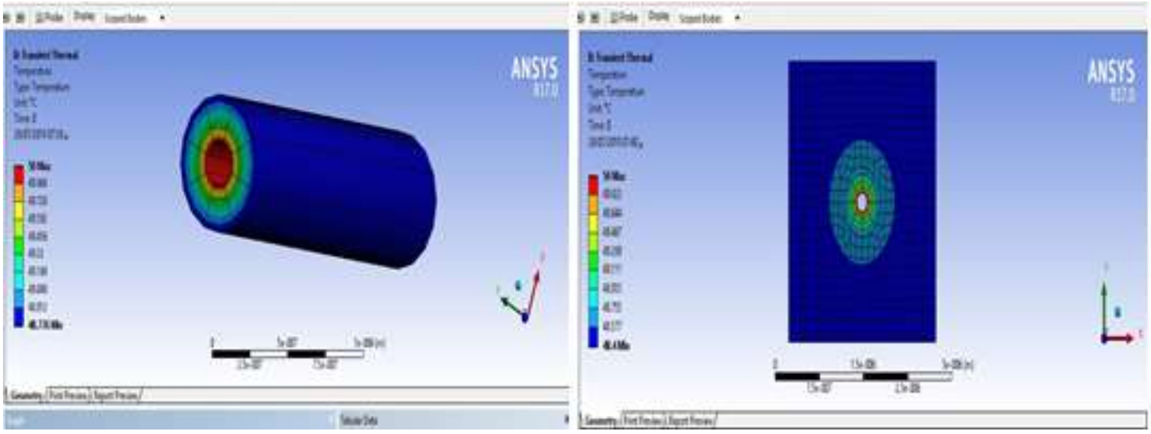


Figure 5: temperature distribution through the carbon nanotube reinforced aluminium matrix

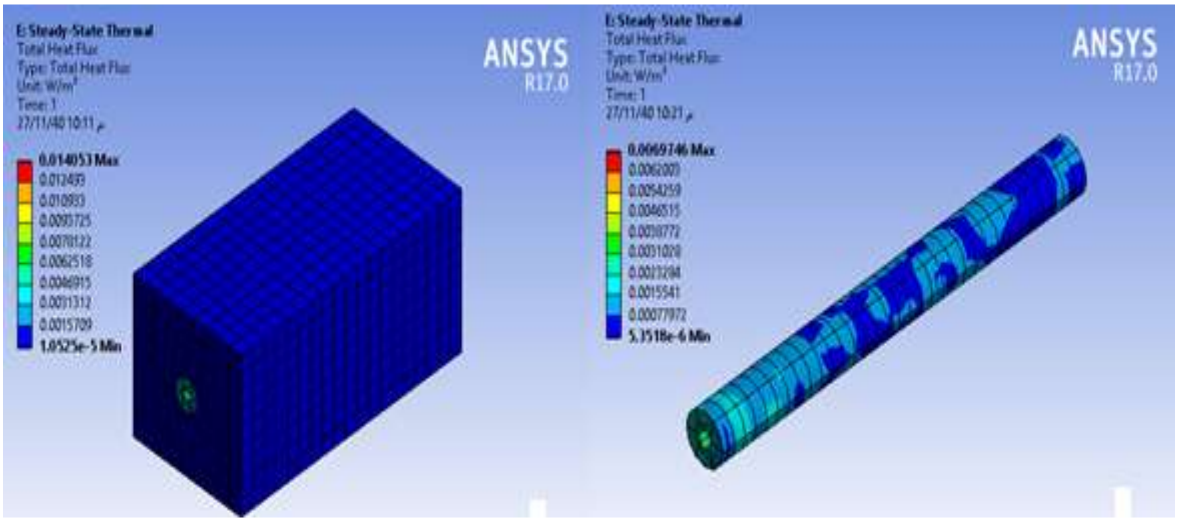


Figure 6: heat flux distribution through the carbon nanotube reinforced aluminium matrix

Validation of thermal conductivity of carbon nanotubes reinforced Aluminium metal matrix Nanocomposite

The finite element results for thermal conductivity of carbon nanotubes reinforced Aluminium metal matrix Nanocomposite was predicted by means of ANSYS-3D model and calculated by the theoretical calculations then compared with the results obtained from different theoretical models [18] as shown in Figure 7. The results show an acceptable agreement and the deviation percentages are calculated for all cases.

It can be observed from the Figures 8, 9 and 10 that the thermal conductivity results of Armchair, Zigzag, and Chiral carbon nanotube treated as long fibre reinforced aluminium matrix have a linear increasing trend with the increase in volume fraction of carbon nanotube. Finite element predictions for the two models show higher value than theoretical results. The deviation percentage were calculated for all cases and presented in Tables 3, 4, and 5.

Table 3: *Validation of thermal conductivity for zigzag carbon nanotube treated as long fibre reinforced aluminium metal matrix*

Vol. (%)	Theoretical (W/m K)	Finite Element (W/m K)	Deviation (%)
3%	221.6	223.3	0.7%
7%	245.1	248.9	1.6%
11%	268.6	274.7	2.3%

Table 4: *Validation of thermal conductivity for zigzag carbon nanotube treated as long fibre reinforced aluminium metal matrix*

Vol. (%)	Theoretical (W/m K)	Finite Element (W/m K)	Deviation (%)
3%	223.6	224.6	0.4%
7%	249.8	252.1	0.9%
11%	275.9	279.5	1.3%

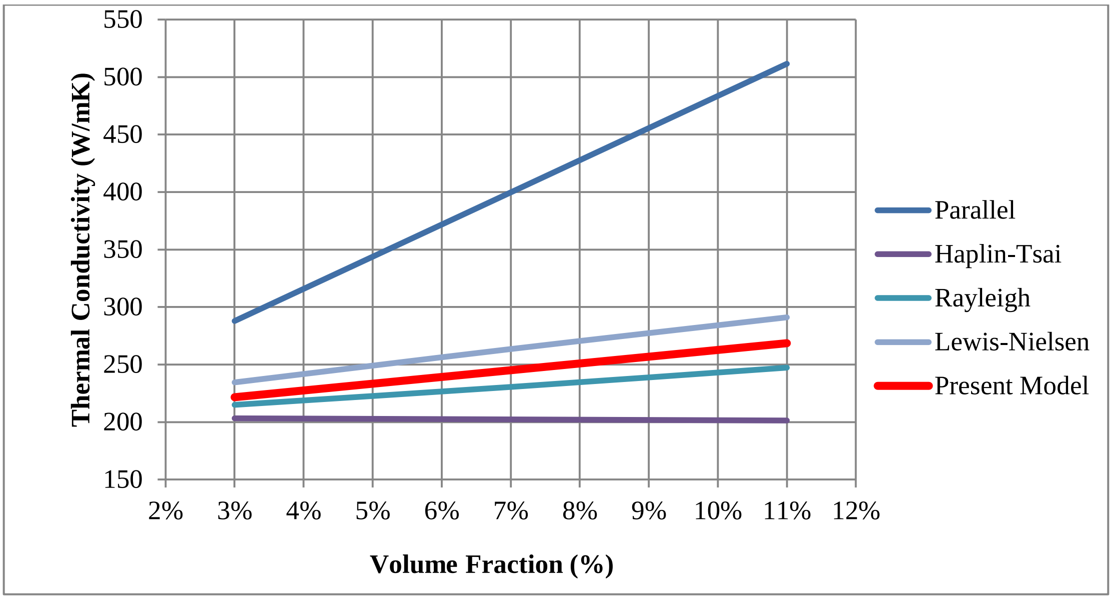


Figure 7: Comparison between the thermal conductivity models for carbon nanotube reinforced aluminum matrix

Table 5: *Validation of thermal conductivity for chiral carbon nanotube treated as long fibre reinforced aluminium metal matrix*

Vol. (%)	Theoretical (W/m K)	Finite Element (W/m K)	Deviation (%)
3%	219.7	222.2	1.1%
7%	240.7	246.5	2.4%
11%	261.6	270.7	3.5%

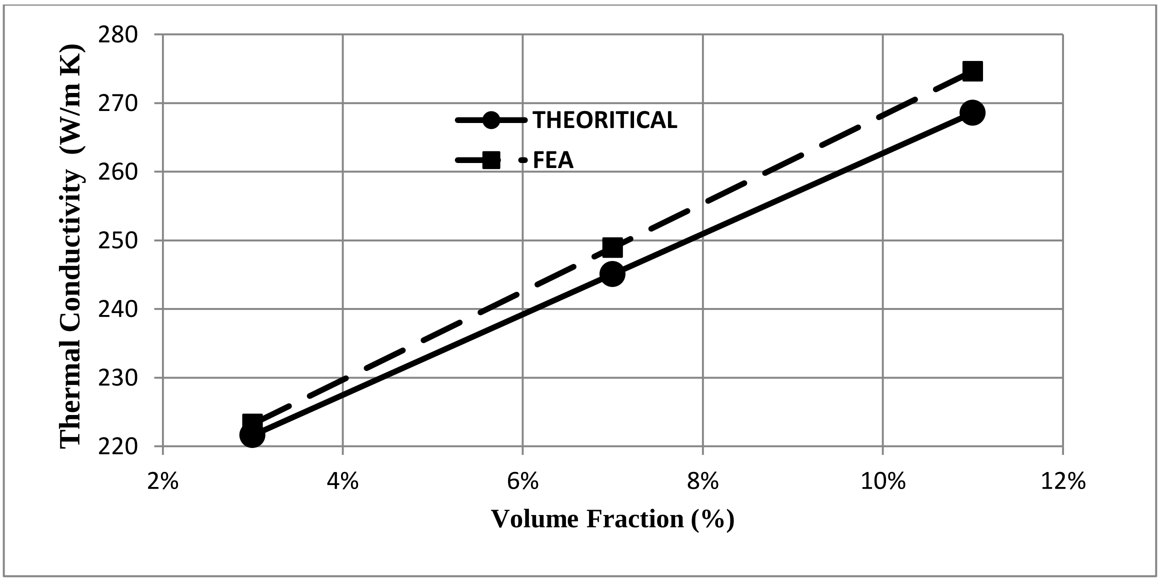


Figure 8: Validation of thermal conductivity for armchair carbon nanotube treated as long fibre reinforced aluminium metal matrix

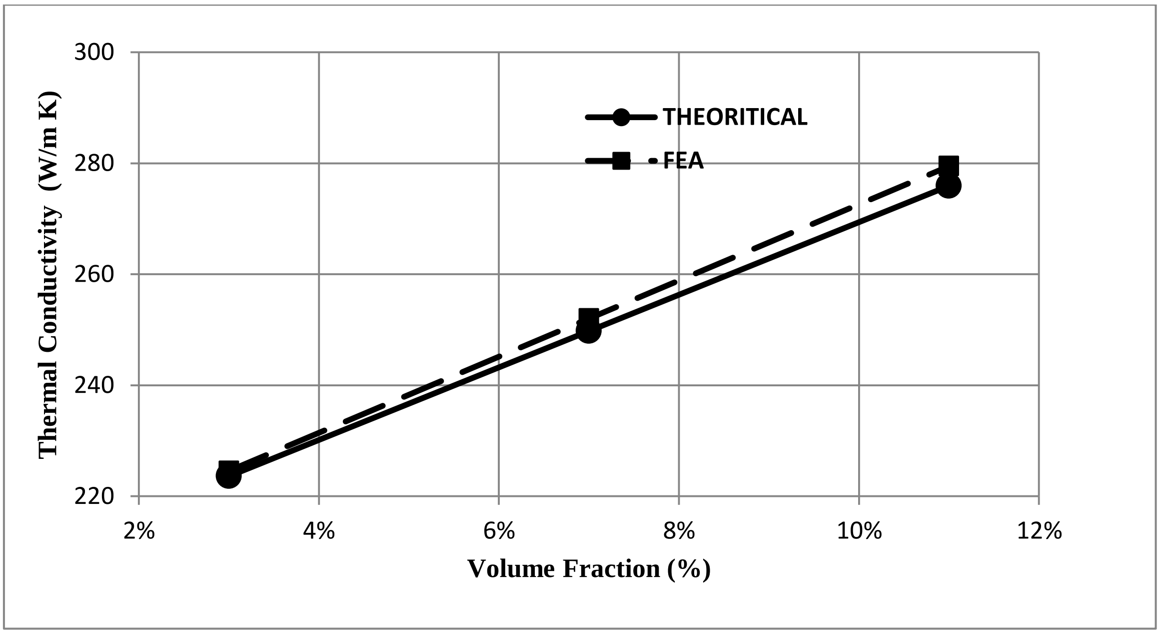


Figure 9: Validation of thermal conductivity for zigzag carbon nanotube treated as long fibre reinforced aluminium metal matrix

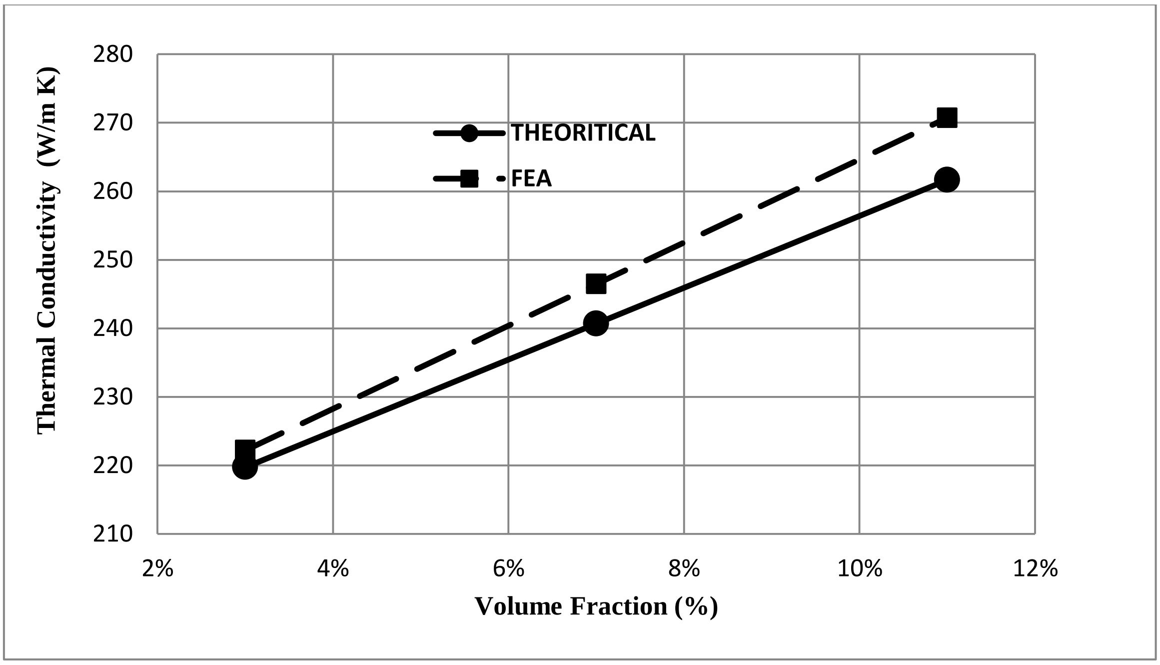


Figure 10: Validation of thermal conductivity for chiral carbon nanotube treated as long fibre reinforced aluminium metal matrix

4. Conclusions

The analysis was carried out with different representative volume element which was modeled for studying specific geometric and material properties. The results obtained were in agreeable range of the theoretical predictions. The finite element analysis of the representative volume elements with same carbon nanotubes and varying volume fractions showed that the effective thermal conductivity varies linearly as predicted with the theoretical model. One of the reasons for getting linear relationship of effective conductivity with the volume fraction is the assumption made during mathematical and finite element modeling of the Nanocomposite that there is no interaction between the neighboring carbon nanotubes.

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