Determination of Elastic Properties of Carbon Nanotubes Treated as Long Fiber for Reinforcing Iron Matrix

G.Goudah
Department of Mechanical Engineering
Sudan University of Science and Technology
Khartoum, Sudan
gehad.hamdan@gmail.com

Suliman, S.M.A.
Department of Mechanical Engineering
University of Bahrain
Sakheer , Bahrain
ssulieman@uob.edu.bh

Elfaki, E. A.
Mechanical Engineering Department
University of Bisha
Bisha, Saudi Arbia
khawad.2002@bu.edu.sa

***Abstract*— in this paper, the effective mechanical properties of carbon nanotubes treated as long fiber based iron metal matrix are evaluated using a 3-D nanoscale representative volum element (RVE) based on continuum mechanics and using the finite element method (FEM). An extended rule of mixtures, based on the strength of materials theory for estimating the effective Young's modulus in the axial direction of the RVE, is applied for comparisons with the numerical solutions based on the elasticity theory. With additions of the carbon nanotubes in a matrix at volume fractions of 3%, 7% and 11%, the stiffness of the composite found to be increased for the carbon nanotube treated as long fiber.**

***Key words*— Carbon nanotubes; Nanocomposites; Effective properties; Representative volume element Finite element method**

I.INTRODUCTION

Current engineering requires the application of new materials with improved properties. This is particularly important in aerospace engineering, high temperature applications, microelectronics, etc., where new composite materials play the basic role in any innovation. Since the discovery of carbon nanotubes [1, 2], researchers have envisioned them promising candidates as reinforcements for composite materials to overcome the performance limits of conventional materials [3, 4], because of their attractive mechanical properties where the stiffness, strength and resilience exceed any current materials. In the past decade, numerous attempts and efforts have been made by researchers, exploiting the exceptional mechanical properties of carbon nanotubes toward the development of carbon nanotubes reinforced composite materials. Polymers, ceramics and metals have been tried out as matrices [5, 6].The primary success lies in polymers reinforced with carbon nanotubes. It was found that the exceptional properties of carbon nanotubes are the consequence of their unique structure. However, the research activity in using carbon nanotubes as reinforcements in metal matrix composites is still scarce, and metal matrix composites reinforced with carbon nanotubes have not yet been developed at a useful scale. Currently, fabrication of carbon nanotube based composites is still a difficult and expensive process. Many basic issues ranging, for example, from characterizations, experimental techniques to simulation methods, have not been fully addressed for the development of CNT-based composites. In the limited number of reports [3, 6], the so-called metal matrix composites are in fact nanoscale composite.[5-8]

One of the requirements in the mechanics of composite materials is to determine the effective elastic properties. At the nanoscale, analytical models are difficult to establish or too complicated to solve, and tests are extremely difficult and expensive to conduct. Modeling techniques like the finite element method are needed to calculate composite material properties, the numerical methods used to estimate composite properties usually involve analysis of a representative volume element (RVE) corresponding to a periodic fiber packing sequence. [9, 10]

The strength of materials (rule of mixtures) approach for estimating the properties of fiber-reinforced composites and the extension of this method to nanocomposite reinforced with long and short carbon nanotubes are investigated to determine the mechanical properties of

the carbon nanotubes reinforced metal matrix nano-composites [11].
In this present paper, 3D nanoscale square representative volume element is employed to investigate the various effects on the elastic properties of carbon nanotubes treated as long fiber reinforced Iron metal matrix and the results of longitudinal modulus (E_L), transverse modulus (E_T), shear modulus (G) and Poisson's ratio (υ) are compared with the rule of mixtures.

II. MATERIALS AND METHODS

1- Rule of Mixture

Simple rules of mixtures can be established based on the strength of materials theory. Rules of Mixtures are mathematical expressions which evaluate some property of the composite in terms of other properties, quantity and arrangement of its constituents.

- Longitudinal Young's Modulus
  $$E_L = E_f * V_f + E_m(1 - V_f) \quad (1.1)$$
- Transverse Young's Modulus
  $$E_T = \frac{E_f E_m}{E_f V_m + E_m V_f} \quad (1.2)$$
- Shear Modulus
  $$G_L = \frac{G_F G_m}{G_F V_m + G_m V_f} \quad (1.3)$$
- Major Poisson's Ratio
  $$v_L = V_f v_f + V_m v_m \quad (1.4)$$

Where,
E_f Elastic modulus of the fiber (GPa)
E_m Elastic modulus of the matrix (GPa)
V_f Fiber volume fraction
G_m Shear Modulus of the Matrix (GPa)
G_F Shear Modulus of the Fiber (GPa)
v_m Major Poisson's Ratio of the Matrix
v_f Major Poisson's Ratio of the Fiber

2- 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.[13, 14]

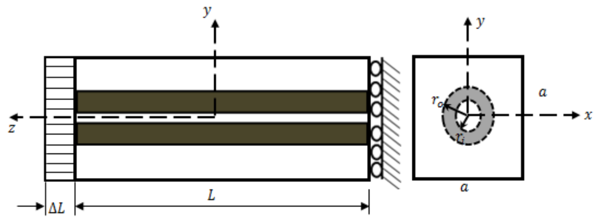

Figure 1: Carbon nanotube through the length of the RVE

$$d_{mean} = \frac{\sqrt{3} * a_{c-c} \sqrt{(m^2)+(m*n)+(m^2)}}{\pi} \quad (2.1)$$

Assuming that thickness of carbon nanotube is 0.34nm

$$d_o = d_{mean} + 0.17 , \quad (2.2)$$

$$d_i = d_{mean} - 0.17 \quad (2.3)$$

Where, d_o and d_i are the outer and inner diameter, respectively.
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

$$V_f = \frac{A_f L}{A_c L} \quad (2.4)$$

$$V_f = \frac{\pi(r_o^2 - r_i^2)}{a^2 - \pi r_i^2} \quad (2.5)$$

Where: V_f = Carbon nanotube volume fraction
a = Width of the square RVE

The mechanical properties for the matrix and reinforcements and the schematic loading, elements and boundary condition of these models are shown in Figure 2 and Table I.

TABLE I: Materials properties

Prperty	Metal Matrix	Reinforcment
	Iron (Steel)	Carbon Nanotube
Density (g/cm^3)	7.85	1.3
Young's Modulus (E) GPa	210	1000
Poisson's Ratio (ϑ)	0.3	0.3
Shear Modulus (G) GPa	82	500

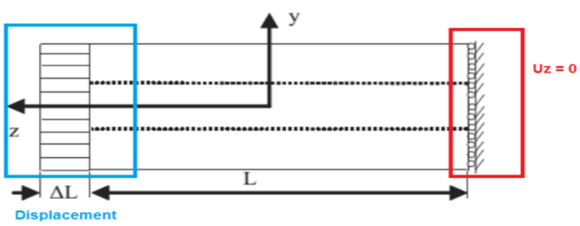

Figure 2: Schematic loading and boundary condition

In order to evaluate the effective properties of composite, the finite element software package ANSYS is used. The program is written in APDL (ANSYS Programming Design Language), which is delivered by the software and it makes the handling much more comfortable. 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. Three-dimensional structural solid element SOLID185 is used to determine elastic properties and is defined by eight nodes having three degrees of freedom at each node: translations in the nodal x, y, and z directions. It also has mixed formulation capability for simulating deformations.

III. RESULTS AND DISCUSSION

1) Density and void fraction

The evaluated theoretical density of the carbon nanotube reinforced iron matrix is shown in Figure. 3. It is observed that the densities have decreasing trend, this may be attributed to increase in the volume fraction of carbon nanotube. It is found that the reduction in the density of the new nanocomposite varied from 1% to 39% when the volume fraction of the carbon nanotubes increased from 1% to 47% for iron matrix

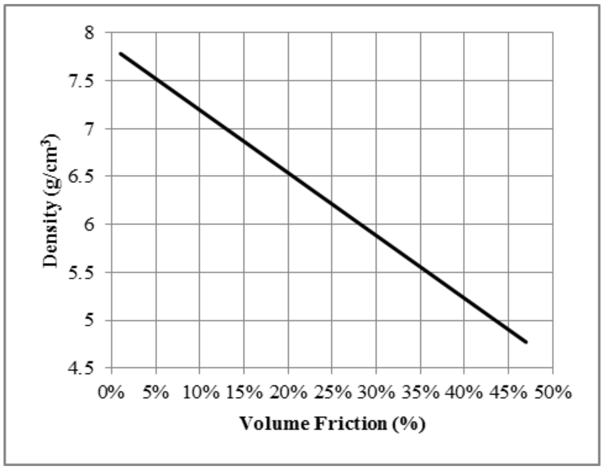

Figure 3: Density for carbon nanotube reinforced iron metal matrix

2) Longitudinal modulus

Longitudinal modulus of composite is the ratio of longitudinal stress to the longitudinal strain. Figure 4 shows the effect of fiber volume fraction on the longitudinal modulus of composites using FEA and rule of mixtures. It can be observed from the Figures 4, 5, and 6 that the longitudinal modulus has increasing trend with the increase in volume fraction of carbon nanotube for different chiral indices and there is good agreement of finite element model with the rule of mixture as presented in Table II.

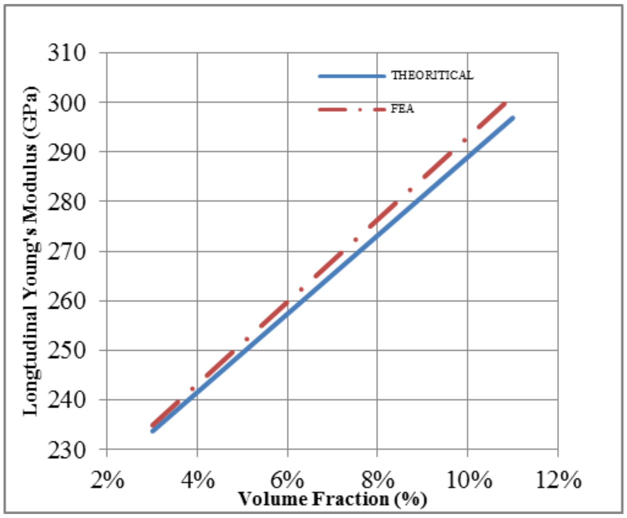

Figure 4: Longitudinal Young's Modulus for Armchair Carbon Nanotube Reinforced Iron metal matrix

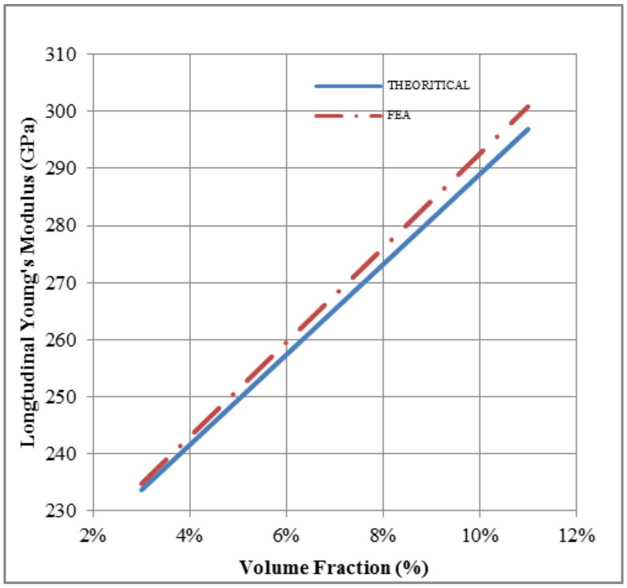

Figure 5: Longitudinal Young's Modulus for Zigzag Carbon Nanotube Reinforced Iron metal matrix

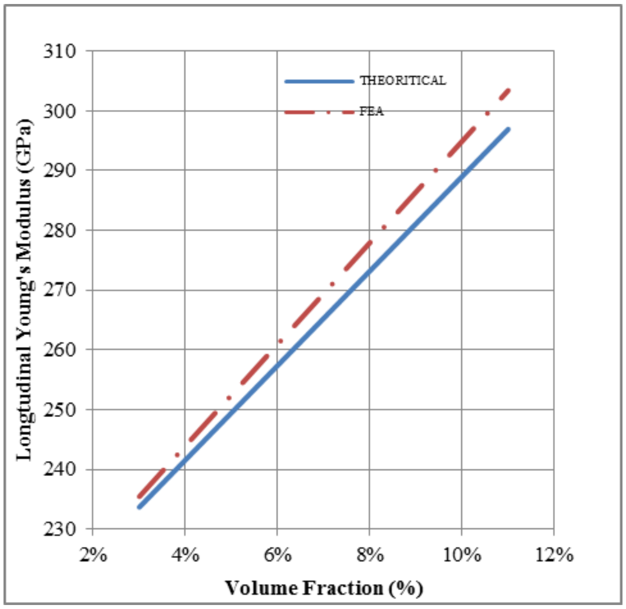

Figure 6: Longitudinal Young's Modulus for Chiral Carbon Nanotube Reinforced Iron metal matrix

3) Transverse modulus

Transverse modulus of composite is the ratio of transverse stress to the transverse strain. Figure 7 shows the effect of fiber volume fraction on transverse modulus of composites using FEA and the rule of mixture. It is clear from the Figures 7, 8, and 9 that the transverse modulus has increasing trend with the increase of carbon nanotube volume fraction. The FEA results are in good agreement with the rule of mixture results as shown in Table III

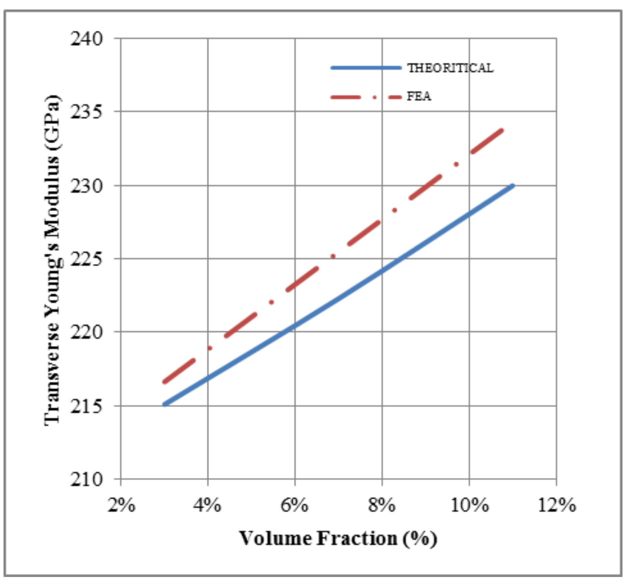

Figure 7: Transverse Young's Modulus for Armchair Carbon Nanotube Reinforced iron metal matrix

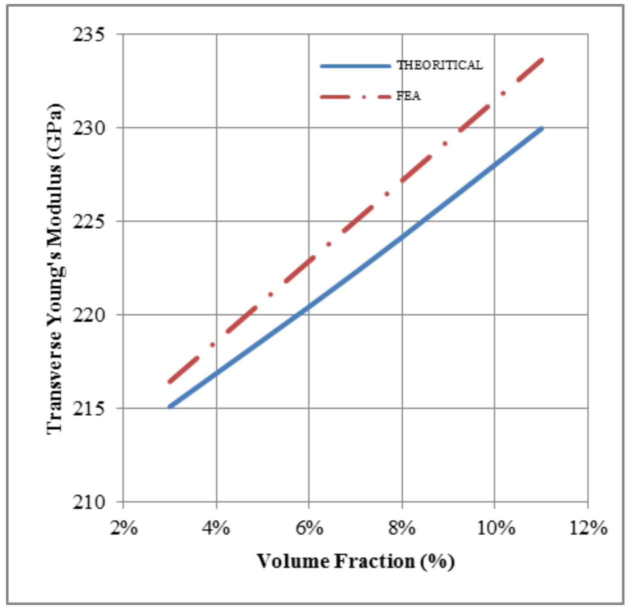

Figure 8: Transverse Young's Modulus for Zigzag Carbon Nanotube Reinforced Iron metal matrix

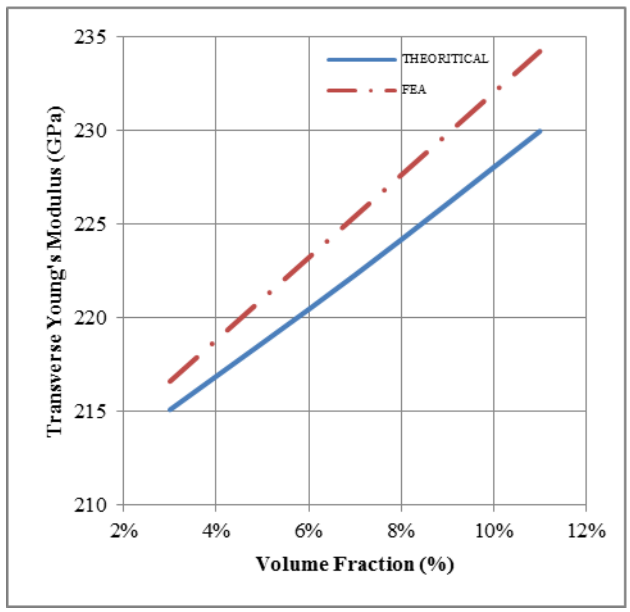

Figure 9: Transverse Young's Modulus for Chiral Carbon Nanotube Reinforced iron metal matrix

4) Shear modulus

Shear modulus of composite is the ratio of shear modulus to the transverse strain. Figures 10, 11, and 12, show the effect of fiber volume fraction on shear modulus of composites using FEA and the rule of mixture. It can be observed that the shear modulus has increasing trend when the volume fraction of carbon nanotube increased. The results are in good agreement for the finite element results compared with the rule of mixture as shown in Table IV

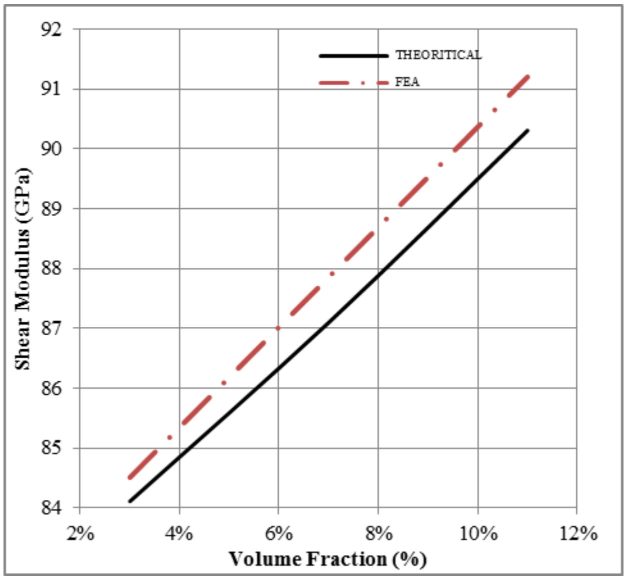

Figure 10: Shear Modulus for Armchair Carbon Nanotube Reinforced iron metal matrix

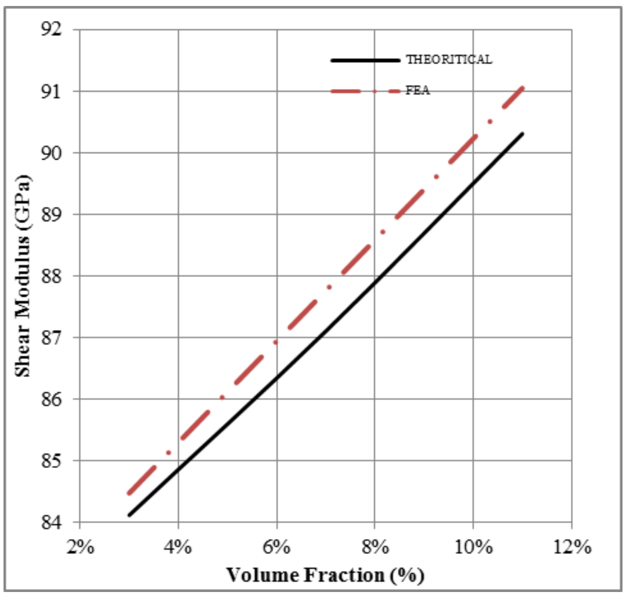

Figure 11: Shear Modulus for Zigzag Carbon Nanotube Reinforced Iron metal matrix

5) Poisson's ratio

The prediction of the major Poisson's ratio for iron matrix reinforced by carbon nanotube does not change as shown in Figure 13 and remains constant through the increments of the volume fraction of the carbon nanotubes because the value of both iron matrix and the carbon nanotube is the same. The results are in good agreement for the finite element results compared to those of rule of mixture.

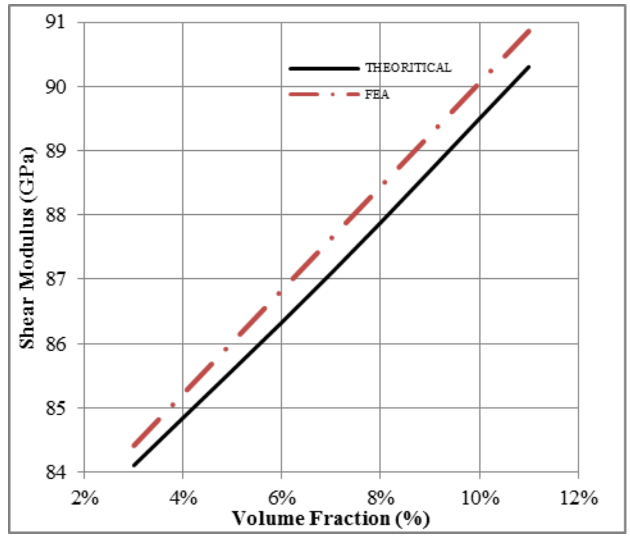

Figure 12: Shear Modulus for Chiral Carbon Nanotube Reinforced iron metal matrix

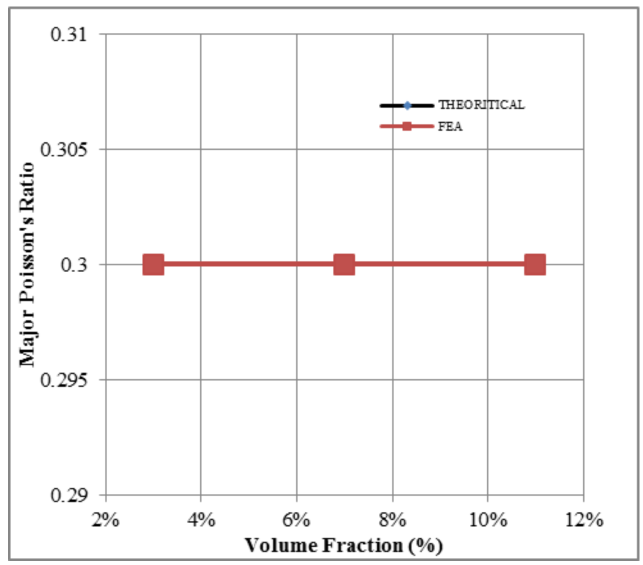

Figure 13: Major Poisson's Ratio for Carbon Nanotube Reinforced Iron metal matrix

IV. CONCLUSIONS

The effective elastic properties of the carbon nanotubes reinforced iron metal matrix nanocomposite were studied using the finite element and theoretical prediction. An ANSYS-APDL macro was used to evaluate the effective elastic properties and they are compared with analytical results based on rule of mixture theory in terms of longitudinal and transverse Young's modulus, shear modulus and major Poisson's ratio. The following conclusions can be drawn:

- Effect of fiber volume fraction on the longitudinal, transverse modulus, and shear modulus of composites is studied. It has been observed that the fiber volume fraction significantly influencing the elastic properties of composites.

TABLE II: Validation of Elastic Properties for Armchair Carbon Nanotube Reinforced Iron Metal Matrix

Volume Fraction (%)	Longitudinal Young's Modulus		Transverse Young's Modulus		Shear Modulus		Percent Deviation (%)		
	Theoretical	FEA	Theoretical	FEA	Theoretical	FEA	E_L	E_T	G
3%	233.7	234.9	215.1	216.84	84.1	84.5	1%	1%	0%
7%	265.3	268.1	222.3	225.96	87.1	87.9	1%	1%	1%
11%	296.9	301.3	230.0	235.08	90.3	91.2	1%	2%	1%

TABLE III: Validation of Elastic Properties for Zigzag Carbon Nanotube Reinforced Iron Metal Matrix

Volume Fraction (%)	Longitudinal Young's Modulus		Transverse Young's Modulus		Shear Modulus		Percent Deviation (%)		
	Theoretical	FEA	Theoretical	FEA	Theoretical	FEA	E_L	E_T	G
3%	233.7	234.78	215.1	216.45	84.1	84.5	0%	1%	0%
7%	265.3	267.82	222.3	225.05	87.1	87.8	1%	1%	1%
11%	296.9	300.86	230.0	233.65	90.3	91.0	1%	2%	1%

TABLE IV: Validation of Elastic Properties for Chiral Carbon Nanotube Reinforced Iron Metal Matrix

Volume Fraction (%)	Longitudinal Young's Modulus		Transverse Young's Modulus		Shear Modulus		Percent Deviation (%)		
	Theoretical	FEA	Theoretical	FEA	Theoretical	FEA	E_L	E_T	G
3%	233.7	235.47	215.1	216.6138	84.1	84.4	1%	1%	0%
7%	265.3	269.43	222.3	225.4322	87.1	87.6	2%	1%	1%
11%	296.9	303.39	230.0	234.2506	90.3	90.9	2%	2%	1%

- Representative volume element model has successfully applied for the finite element analysis using ANSYS software. The numerical results agreed with the existing analytical predictions

REFRENCES

1 Iijima, S.: ‘Helical Microtubules of Graphitic Carbon’, Nature 1991, 354, pp. 56-58

2 Iijima, S., and Ichihashi, T.: ‘Single-Shell Carbon Nanotubes of 1-Nm Diameter’, Nature, 1993, 363, pp. 603-605

3 Baughman, R.H., Zakhidov, A.A., and Heer, W.A.d.: ‘Carbon Nanotubes-the Route Toward Applications ’, Science, 2002, 297, (5582), pp. 787-792

4 Thostenson, E.T., Ren, Z., and Chou, T.-W.: ‘Advances in the science and technology next term of carbon nanotubes and their previous term composites:next term a review’, Composites Science and Technology, 2001, 61, (13), pp. 1899-1912

5 Sinnott, S.B., and Andrews, R.: ‘Carbon nanotubes: synthesis, properties, and applications’, Critical Reviews in Solid State and Materials Sciences, 2001, 26, (3), pp. 145–249

6 Chen, X., Xia, J., Peng, J., Li, W., and Xie, S.: ‘Carbon-nanotube metal-matrix composites prepared by electroless plating ’, Composites Science and Technology, 2000, 60, (3), pp. 301-306

7 Agarwal, A., Bakshi, S.R., and Lahiri, D.: ‘Carbon Nanotubes Reinforced Metal Matrix Composites’ (CRC Press,Taylor & Francis Group, 2011)

8 Jorio, A., Dresselhaus, G., and Dresselhaus, M.S.: ‘Carbon Nanotubes:Advanced Topics in the Synthesis, Structure, Properties and Applications’ (Springer Science+Business Media, 2008)

9 Li, S.: ‘General Unit Cell for Micromechanical Analyses of Unidirectional Composites,’ Composites Part A, 2000, 3, (6), pp. 815-816

10 Kim, B.R., and Lee, H.K.: ‘An RVE-Based Micromechanical Analysis of Fiber-Reinforced Composites Considering Fiber Size Dependenc’, Composite Structures, 2009, 90, (4), pp. 418-427

11 Agarwal, B.D., Broutman, L.J., and Chandrashekhara, K.: ‘Analysis and Performance of Fiber Composites’ (John Wiley & Sons., 2006, 3rd edn.)

12 Rémond, Y., Ahzi, S., Baniassadi, M., and Garmestani, H.: ‘Applied RVE Reconstruction and Homogenization of Heterogeneous Materials ’ (John Wiley & Sons, Inc. and ISTE Ltd 2016)

13 Islam, M.S., and Szpunar, J.: ‘Effects of Orientation of Carbon Nanotubes on CNT Bundle Based Silk Composite Using Finite Element Method’, Modeling and Numerical Simulation of Material Science, 2013, (3), pp. 33-38

14 Islam, M.S., Riktan, F.O., Chowdhury, S.C., Chowdhury, M.M.R., and Ahmed, S.: ‘Evaluation of Tensile Modulus of Carbon Nanotube Bundle Based Composite with Interface Using Finite Element Method’. Proc. 2011 COMSOL Conference, Banglore.