DETERMINATION OF THE MECHANICAL PROPERTIES OF CARBON NANOTUBES REINFORCED ALUMINUM MATRIX TREATED AS LONG FIBER USING FINITE ELEMENT ANALYSIS

Gehad. G. Hamdan
Faculty of Petroleum Engineering,
University of Al-Jufra,
Zellah, Libya
gehad.hamdan@gmail.com

ABSTRACT

In this paper, the effective mechanical properties of carbon nanotube treated as long fiber reinforced Aluminum metal matrix are evaluated using a 3-D nanoscale representative 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 expected to be increased for the carbon nanotube treated as long fiber. The results show that, the finite element results varies between 3 to 28% lower than the theoretical one for the longitudinal young's modulus (**E_L**) and between 0.05 to 0.17 for Poisson's Ratio **(ϑ)**. However, the FEA results varies between 3 to 5% and 1 to 3% for transverse young's modulus **(E_T)** and shear modulus **(G)**.

Keywords: Carbon nanotubes; Nano composites; Effective properties; Representative volume element (RVE), Finite element method

INTRODUCTION

Composite materials can be derived from two or more constitutes to form other different materials have different properties. However, Nano composite materials have been attracting major attention because of their promise in developing extremely strong materials and the basic opportunities they present. Although there have been many advancements in the manufacturing of Nano composite materials, thus far, these processes have only been moderately successful in producing isotropic properties in polymer reinforced Nano composite matrices.[1-3]

Aluminum is one of the most studied structural materials in the last years to produce MMC due to its large use in different industrial sectors like: aeronautical, nautical and automotive in which the low weight of vehicles is very important. However, it is expected that the Aluminum composites with carbon nanotubes reinforcement would possess better tensile and compressive properties compared to pure Aluminum. The hardness of the obtained composites is also expected to be greater than that of pure aluminum. The Al-CNT composite is found to be affluent in improving the mechanical properties such that even for a small amount of CNT addition the response ineffective. [2-4]

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. [4- 6]

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 [6- 8].

In this 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.

MATERIALS AND METHODS

Rule of Mixture

Simple rules of mixtures can be established based on the strength of materials theory. Rules of Mixtures are mathematical expressions [6, 11-14] which evaluate some property of the composite in terms of other properties, quantity and arrangement of its constituents.

- Longitudinal Young's Modulus

$$E_L = E_f * V_f + E_m(1 - V_f) \quad (1)\ [6, 11\text{-}13]$$

- Transverse Young's Modulus

$$E_T = \frac{E_f E_m}{E_f V_m + E_m V_f} \quad (2)\ [6, 11\text{-}13]$$

- Shear Modulus

$$G_L = \frac{G_F G_m}{G_F V_m + G_m V_f} \quad (3)\ [6, 11\text{-}13]$$

- Major Poisson's Ratio

$$v_L = V_f v_f + V_m v_m \quad (4)\ [6, 11\text{-}13]$$

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

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[9]. The RVE used for analyzing long carbon nanotube reinforced Aluminum 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 and the dimensions are given in Table 1. The diameter of the carbon nanotube is varied according to the chiral indices Armchair, Zigzag, and Chiral ((10, 10), (10, 0), (10, 15)), respectively. The mean diameter (d_{mean}) of the CNT is obtained from this chiral index.[16, 17]

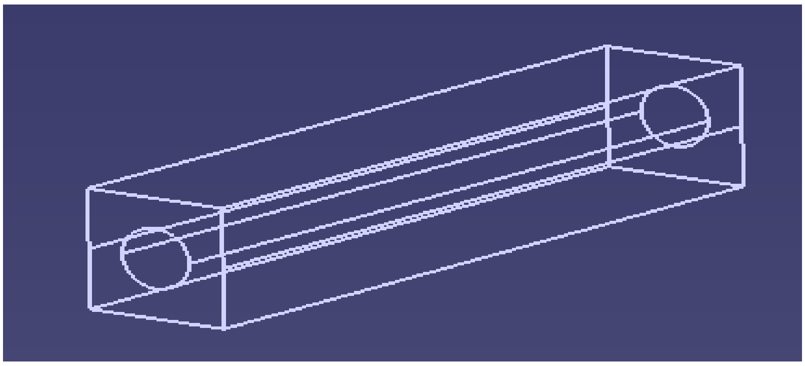

FIGURE 1: Carbon nanotube through the length of the RVE

TABLE 1: Dimensions for long fiber case

Type of CNT	**CNT**		**D_o**	**D_i**	**a (width of square RVE)**		
	N	**M**			**v_f=3%**	**v_f=7%**	**v_f=11%**
Armchair CNT	10	10	1.526	1.186	6.8898	5.3418	3.5152
Zigzag CNT	10	0	0.953	0.613	5.2650	4.0986	2.7291
Chiral CNT	10	15	1.876	1.536	7.6996	5.9536	3.8862

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

$$V_f = \frac{A_f L}{A_c L} \qquad (5)\ [6, 11\text{-}13]$$

$$V_f = \frac{\pi(r_o^2 - r_i^2)}{a^2 - \pi r_i^2} \qquad (6)\ [6, 11\text{-}13]$$

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 2.

TABLE 2: Materials properties

Prperty	Metal Matrix	Reinforcment
	Aluminum	Carbon Nanotube
Density (g/cm^3)	2.712	1.3
Young's Modulus (E) GPa	70	1000
Poisson's Ratio (ϑ)	0.33	0.3
Shear Modulus (G) GPa	26	500

In order to evaluate the effective properties of composite, the finite element software package ANSYS is used. A 3D finite element model where the length of the carbon nanotubes is equal to the length of the RVE was constructed to study its elastic moduli; this model was built in by parametric as the APDL code (script) [15, 16]. The code is transferred to ANSYS for computational modeling. 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 [17] 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.

RESULTS AND DISCUSSION

The finite element results for elastic properties of carbon nanotubes reinforced metal matrices Nanocomposite was determined by means of ANSYS-APDL macro and compared with the results obtained by MATLAB code based on rule of mixture theory.

The finite element results show an acceptable agreement compared with the theoretical results. The deviation percentage were calculated and presented. It can be observed from the Figures 2, 3 and 4 that the elastic property results for carbon nanotube reinforced aluminum matrix have an increasing trend with the increase in volume fraction of carbon nanotube for different chiral indices while Figure 5 shows decreasing trend for major Poisson’s ratio.

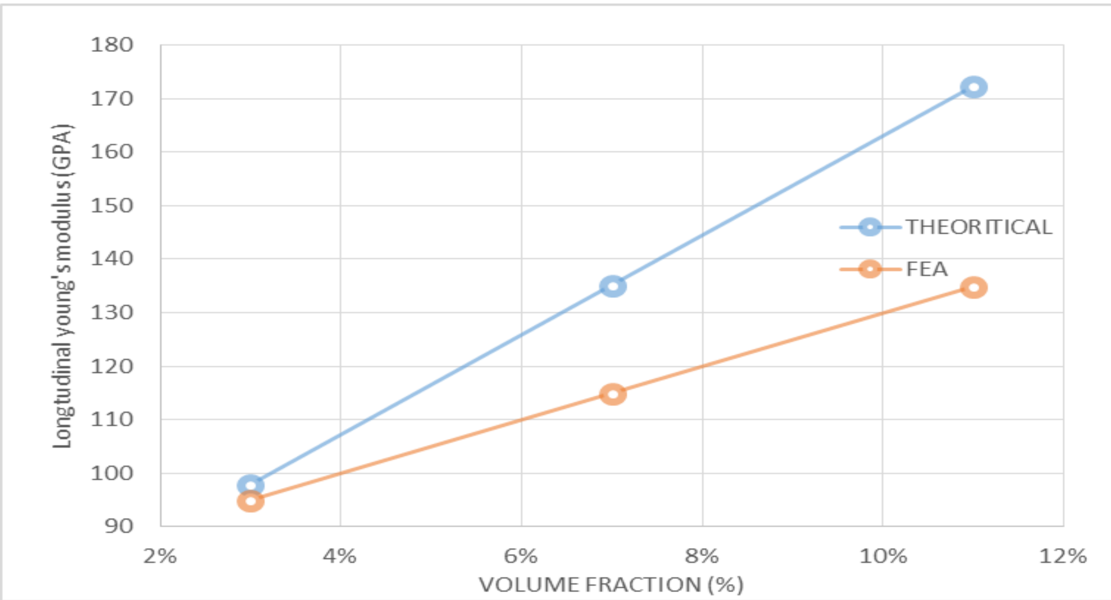

Figure 2: **Longitudinal Young's modulus for CNT reinforced Aluminum metal matrix validation**

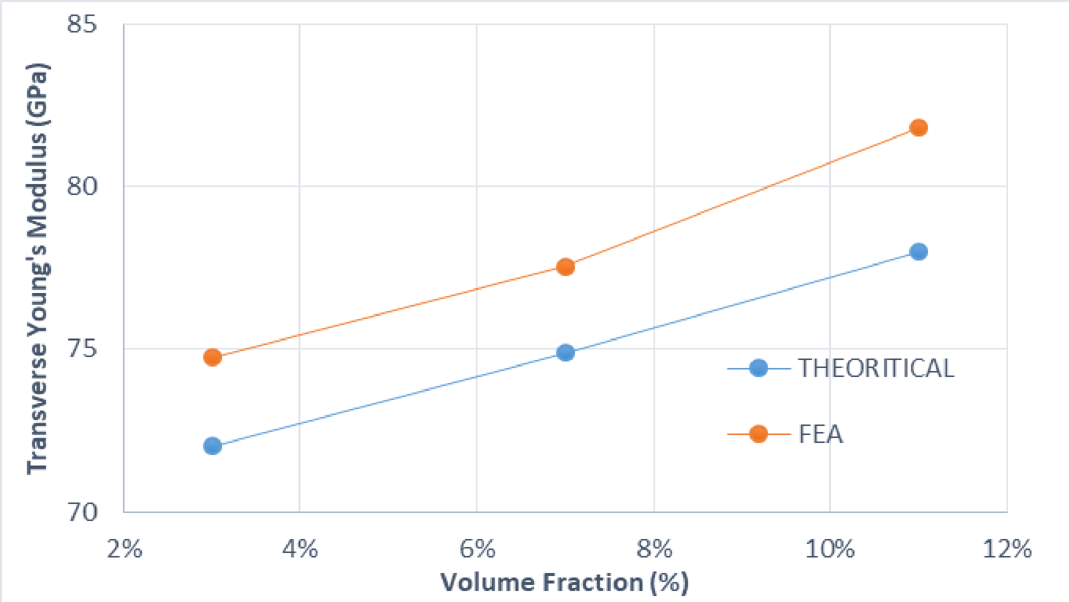

Figure 3: Transverse modulus for CNT reinforced Aluminum metal matrix validation

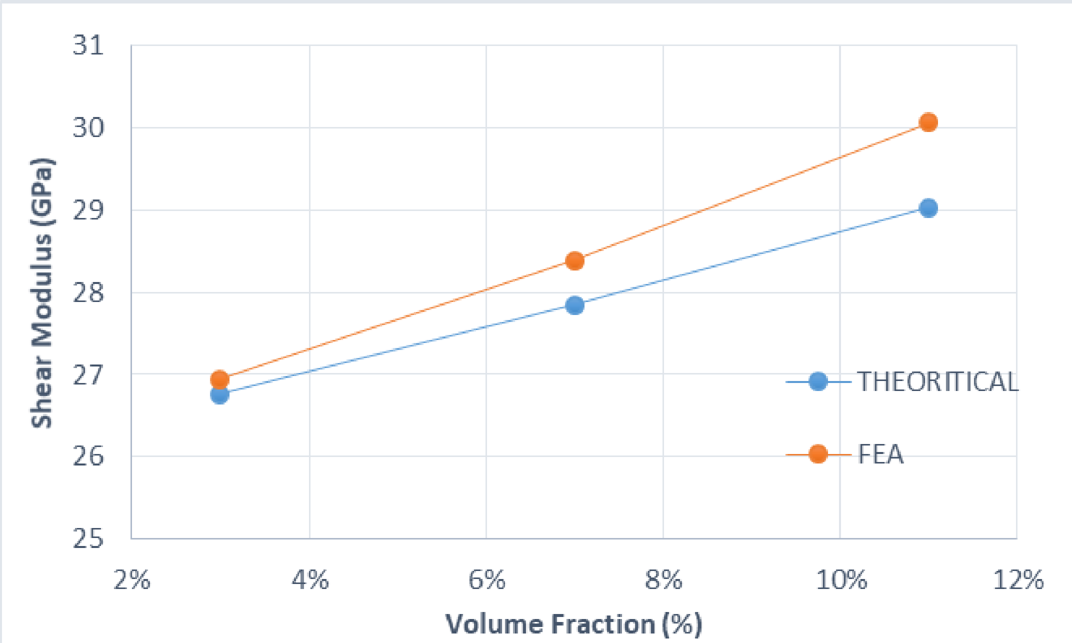

Figure 4: Shear modulus for CNT reinforced Aluminum metal matrix validation

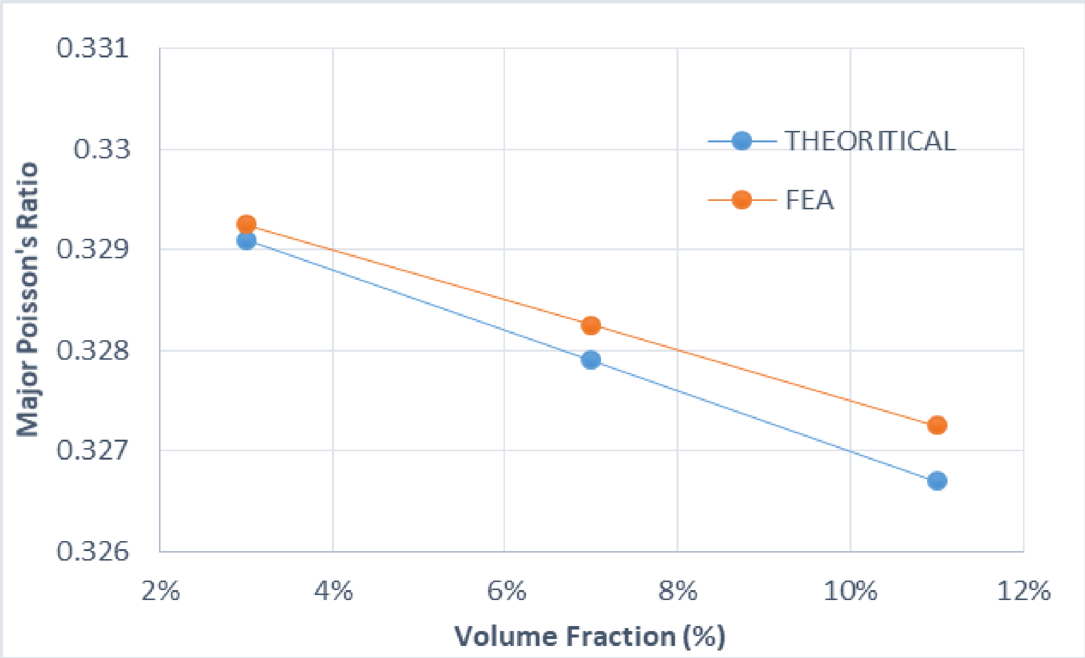

Figure 5: Major Poisson's ratio CNT reinforced Aluminum metal matrix validation

The results are in good agreement for the finite element results compared to those of rule of mixture. The validation of the results obtained for longitudinal young's modulus, transverse modulus, shear modulus and major Poisson's ratio as presented in Table 3, 4, 5 and 6 respectively. It appears that, the finite element results varies between 3% and 28% lower than the theoretical one for the longitudinal young's modulus (**E_L**) and between 0.05% and 0.17% for Poisson's Ratio **(ϑ)**. However, the FEA results varies between 3% to 5% and 1% to 3% for transverse young's modulus **(E_T)** and shear modulus **(G)**

Table 3:Validation of Longitudinal Young's Modulus (E_L GPa) for CNT reinforced Aluminum Metal Matrix

Vol. (%)	Longitudinal Young's Modulus (E_L *GPa)*		Percent Deviation (%)
	Theoretical	FEA	E_L
3%	97.9	94.96	-3%
7%	135.1	114.91	-18%

11%	172.3	134.86	-28%

Table 4:Validation of Transverse Young's Modulus (E_T *GPa*) for CNT reinforced Aluminum Metal Matrix

Vol. (%)	Transverse Young's Modulus (E_T *GPa*)		Percent Deviation (%)
	Theoretical	FEA	E_T
3%	72.01	74.74	4%
7%	74.87	77.54	3%
11%	77.98	81.79	5%

Table 5:Validation of shear Modulus (G *GPa*) for CNT reinforced Aluminum Metal Matrix

Vol. (%)	Shear Modulus (G *GPa*)		Percent Deviation (%)
	Theoretical	FEA	G
3%	26.76	26.9	1%
7%	27.85	28.4	2%
11%	29.03	30.1	3%

Table 6:Validation of Poisson's Ratio (ϑ) for CNT reinforced Aluminum Metal Matrix

Vol. (%)	Poisson's Ratio (ϑ)		Percent Deviation (%)
	Theoretical	FEA	ϑ
3%	0.3291	0.32925	-0.05%
7%	0.3279	0.32825	-0.11%
11%	0.3267	0.32725	-0.17%

CONCLUSIONS

The effective elastic properties of the carbon nanotubes reinforced Aluminum 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 finite element results show lower variation than the theoretical one for the longitudinal young's modulus (**E_L**) and for Poisson's Ratio **(ϑ)**. However, the FEA results show higher variation than the theoretical one for transverse young's modulus **(E_T)** and shear modulus **(G)**.

The following conclusions can be drawn:

- The results are in good agreement for the finite element results compared to those of rule of mixture.
- 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.
- Representative volume element model has successfully applied for the finite element analysis using ANSYS software. The numerical results agreed with the existing analytical predictions

REFERENCES

[1] Rafiei, S.: 'Foundations of Nanotechnology: Mechanics of Carbon Nanotubes' (Apple Academic Press, Inc, 2015)

[2] Shuai Zhang, Gaoqiang Chen, Timing Qu, Jinquan Wei, Yufan Yan, Qu Liu, Mengran Zhou, Gong Zhang, Zhaoxia Zhou, Huan Gao, Dawei Yao, Yuanwang Zhang, Qingyu Shi & Hua Zhang: " A novel aluminum-carbon nanotubes nanocomposite with doubled strength and preserved electrical conductivity" Nano Research volume 14, pages2776–2782 (2021)

[3] Danilo Marini, Virgilio Genova , Francesco Marra, Giovanni Pulci, Marco Valente:" Mechanical Behaviour with Temperatures of Aluminum Matrix

Composites with CNTs" Chemical Engineering Transactions, Vol. 60, 2017,pp.: 25-30
[4] Hu, N.: 'Composites and Their Properties' (InTech, 2012)
[5] Preethi.K, Raju T.N, Shivappa H.A:" Development and Characterization of Carbon Nanotube Reinforced Aluminium-6061 Metal Matrix Composites" Journal of Minerals and Materials Characterization and Engineering, 2021, 9, 290-300
[6] Joseph Kuruvilla Kristiina Oksman George Gejo Runcy Wilson Saritha Appukuttan:" Fiber Reinforced Composites, Constituents, Compatibility, Perspectives and Applications" 1st edition, Woodhead Publishing, 2021
[7] Sohail M. A. K. Mohammed, Daolun L. Chen:" carbon nanotube-reinforced aluminum matrix composite" Advanced Engineering MaterialsVolume 22, Issue 4, 2019
[8] Kim, B.R., and Lee, H.K.: 'An RVE-Based Microme- chanical Analysis of Fiber-Reinforced Composites Con- sidering Fiber Size Dependenc', Composite Structures, 2009, 90, (4), pp. 418-427
[9] 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)
[10] Bedri Onur Kucukyildirim, Aysegul Akdogan Eker:" Fabrication of carbon nanotube reinforced aluminum alloy composites by vacuum-assisted infiltration technique" Journal of Composite Materials, Vol 55, Issue 16, 2021
[11] 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
[12] 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.
[13] Philippe Boisse:" Composite Reinforcements for Optimum Performance" 2nd edition, Woodhead Publishing, 2020
[14] Fan, C.-W., Huang, J.-H., Hwu, C., and Liu, Y.-Y.: 'Mechanical Properties of Single-walled Carbon Nanotubes - A Finite Element Approach', Advanced Materials Research, 2008, 33-37, pp. 937-942
[15] Lee, H.-H.: 'Finite Element Simulations with ANSYS Workbench 14' (SDC Publications, 2012)
[16] Alawadhi, E.M.: 'Finite Element Simulations Using ANSYS' (CRC Press 2010)
[17] Chen, X., and Liu, Y.: 'Finite Element Modeling and Simulation with ANSYS Workbench' (CRC Press 2015)