International Journal of Applied Engineering Research ISSN 0973-4562 Volume 13, Number 6 (2018) pp. 263-267
© Research India Publications. http://www.ripublication.com

Modeling of Elastic properties of Particulate Composites

Ajay Kumar
Department of Mechanical Engineering,
KIET Group of Institutions, Ghaziabad, India

Dr. Sachin Kumar Singh
Department of Mechanical Engineering,
I. I. T. Dhanbad, India

Dr. Subodh Sharma
Department of Mechanical Engineering,
KIET Group of Institutions, Ghaziabad, India

Dr. Arunesh Chandra[1]
Department of Mechanical Engineering,
KIET Group of Institutions, Ghaziabad, India

Abstract

In this present work the effective elastic modulus of nanocomposites of epoxy reinforced with spherical shape Al_2O_3 particles of 40 nanometer diameter, up to a volume fraction of 10%, randomly distributed, is evaluated under uniaxial loading condition using finite element method (FEM). In order to obtain realistic prediction of elastic modulus of polymer nanocomposites, three dimensional representative volume elements (RVE) were considered. A MATLAB code was written to position the particles inside the RVE randomly. The ANSYS Parametric Design Language (APDL) of the software was used to generate the RVE and evaluate the elastic modulus. Five different RVEs were analyzed and the average of elastic modulus from the five analyses was taken for final result for each volume fraction of alumina particles.

Elastic modulus of polymer nanocomposites obtained from the finite element analysis was also compared with the result obtained from Halpin Tsai analytical model, and the possible reasons of deviations between the two results are discussed. It was found that the elastic modulus of polymer nanocomposite having 10% volume fraction increased by an amount of 26% over that of neat epoxy.

Keywords: Nanocomposites, modeling of material, particulate composite, elastic modulus.

Introduction

Nanocomposites are multiphase solid material where one of the phases has one, two or three dimensions of less than 100 nanometers (nm), or structures having nano-scale repeat distances between the different phases that make up the material. Due to extremely low size and high aspect ratio, nano particles have become ideal reinforcement to improve the mechanical and electrical properties of polymer matrix. In comparison to metals polymers have very less elastic modulus as well as resistance to fracture or crack growth. Nano particles improve the elastic modulus and fracture toughness of polymer even at low volume substantially.

Determination of effective elastic properties of polymer nanocomposite material is a typical problem in solid mechanics. There are many analytical and semi analytical techniques to evaluate effective mechanical properties of nanocomposites. There are a number of classical micro-mechanical theories which have been reported in the literature. The Voigt and Reuss approximation model are the simplest models used to evaluate the effective properties of a composite. But neither Voigt nor Reuss model predict accurate effective properties of composite. In Voigt model the stresses across the boundaries of the phases do not follow equilibrium equation, and in the Reuss model the resulting strains create forces to debond the phases **[1, 2]**. Hashin–Shtrikman's variational principles established the upper and lower bounds for elastic modulus of composite **[3]**. Eshelby has considered an ellipsoidal inclusion in an infinite isotropic matrix to solve the problem of particulate composites **[4]**. Eshelby realized that problem should be equivalent to the problem of a region in a matrix with different material properties. Effective field theory based on Eshelby's has been used by Mori–Tanaka to find the elasticity solution for inhomogeneity in infinite medium **[5]**. Benveniste reformulated it so that it could be applied to composite materials **[6]**. Halpin-Tsai model is based on the geometry and orientation of the reinforcement and the elastic properties of the reinforcement and matrix. The model is based on the self consistent field method although often consider to be empirical **[7]**. Halpin –Tsai and Mori-Tanaka are two most popular analytical models for evaluation effective elastic properties of micro/nano composite have been found in literature..

A lot of work has been reported for evaluating the effect of nano-reinforcement on elastic modulus of polymers experimentally **[8-13]**. Limited availability of literature which deals with modeling of randomly distributed nano meter size reinforced composite motivated the present work. Unit cell model **[14]** was being used for evaluating the properties of fiber reinforced polymers. To simulate different volume fractions the size of matrix is kept fixed while the radius of spherical inclusion is varied. All the unit cell model simplifies the material as a periodic array of reinforcement. These models have the limitation that reinforcements are assumed to have same shape and orientation. But in real composites, there are variation in size, distribution and orientation of particles in the matrix. To overcome these problems Nemat-Naseer used a Representative Volume Element approach **[18]**. The volume of the RVE should be chosen in such a way that the RVE contains adequate number of reinforcement to represent the composite statistically.

Marur [14] have modeled composites of epoxy reinforced with spherical glass particles. Unit cell models are employed to model the composite. Three unite cell; Cylindrical, Spherical, and cubical shape with spherical inclusion were taken to evaluate the effective elastic properties. The results were compared with analytical model (TPM) and with experimental results. **Kari et al [15]** evaluated the effective material properties (E, G, K and ν) of micro-composites by RVE approach based on finite element method with periodic boundary conditions for volume fraction from 10% to 60% of particles. Random Sequential Adsorption algorithm (RSA) was used to generate three dimensional RVE model with randomly distributed spherical particles. **Hbaied et al [16]** modeled elastic Modulus of Epoxy/Nanoclay nanocomposite with square plate for aligned particle and disc shape for randomly oriented particle. Finite element analysis was carried out for two dimensional and three dimensional RVE on ABAQUS. Randomly oriented particles could not be randomly distributed at high volume fraction. Both the epoxy and clay were taken as isotropic and linearly elastic. For aligned particles, Mori-Tanaka model is reasonably accurate up to 5% volume fraction of nano clay but underestimates the stiffness at higher volume fractions. For randomly oriented particles, the Mori-Tanaka model overestimates the stiffness of clay nanocomposite. **Parameswaran and Shukla [17]** evaluated the effective elastic modulus of nanocomposite of epoxy/Alumina platelets, with RVE approach using finite element method. Finite element simulation was performed on ANSYS 8. Four RVE configuration Uniform Size Aligned Platelets (USAP), Assorted Size Aligned Platelets (ASAP), Uniform Size Randomly Oriented (USRO), Assorted Size Randomly Oriented (ASRO) is considered. Size of RVE is determined by varying size by 15 to 30µm for composite having 1% VF of aligned platelets. The effect of Four RVE configuration on elastic Modulus is investigated and found that ASRO is most close to experimental value. Result is also compared with Mori Tanaka method.

Methods

2 Modeling of Nanocomposite

2.1 Material system

In the present work, epoxy has been taken as matrix material and alumina particles of spherical shape of 40nm diameter have been taken as reinforcement. For epoxy, the elastic modulus and Poisson's ratio is taken as 3.8 GPa and 0.375 respectively. The elastic modulus of alumina particles is taken as 375 GPa and the Poisson's ratio is 0.23.

2.2 Finite element modeling and boundary conditions

A MATLAB code was written to position the particles inside the RVE randomly. It was ensured that the closest distance between two particles is not less than 40 nm. Five different RVEs were analyzed and the average of elastic modulus from the five analyses was taken for final result for each volume fraction of alumina particles.

The stress strain behavior of nanocomposites was modeled on nano scale using the finite element program ANSYS. The ANSYS Parametric Design Language (APDL) of the software was used to generate the RVE. The two dimensional (2D) and three dimensional (3D) figure of RVE on which analysis was performed are shown in **Fig 1 and Fig 2**.

In most modern papers in the field of strategic management the concept of competitive strategy is interpreted as a set of rules and practices to be followed by the enterprise, if its purpose is to achieve and maintain the competitiveness in the industry [2, 3, 4, 5, 6, 7, 8, 9]. Therefore, the competitive strategy of the enterprise is focused on achieving the competitive advantages, ensuring the best possible and sustainable long-term financial position as well as the strong position in the market.

M. Meskon, M. Albert, F. Hedouri defined the strategy as "a detailed comprehensive and integrated plan designed to ensure the implementation of the mission of the enterprise and its objectives" [10]. The strategic planning process in general can be represented by the following algorithm (Figure 1).

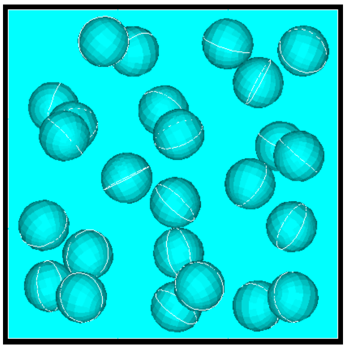

Figure 1: 2D figure of RVE of composite having 5%

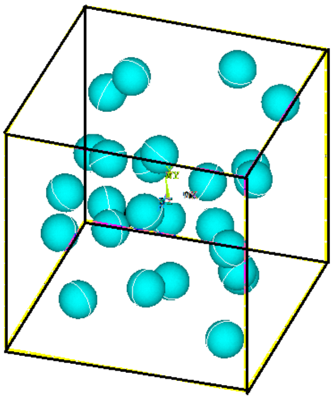

Figure 2: 3D figure of RVE of composite having 5%

Ten nodded tetrahedral elements were used to mesh both the matrix and the platelets. This corresponds to the SOLID187 ANSYS element. The number of elements varied from 25,000 to 350,000 depending on the volume fraction used. A RVE with finite element mesh is shown in **Fig 3.** Prescribing periodic boundary conditions is difficult with randomly oriented reinforcements, especially while performing a three-dimensional analysis. Further, it is reported that the effect of symmetric boundary conditions or periodic boundary conditions on the evaluated elastic modulus is negligible **[16]**. Hence relatively simpler symmetric boundary conditions were prescribed in the present study. The displacement components normal to the three adjacent faces of the RVE were constrained to prevent rigid body motion. All the nodes on remaining two faces were coupled to remain faces parallel during deformation. A normal displacement of known value was applied to the nodes on the sixth face. The stress was calculated by dividing the total reaction obtained from the finite element result by cross sectional area of RVE. The elastic modulus was calculated by dividing the stress by the applied strain.

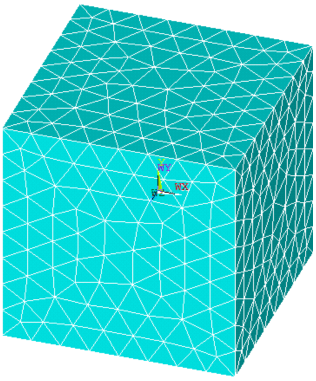

Figure 3: Finite element meshing of RVE

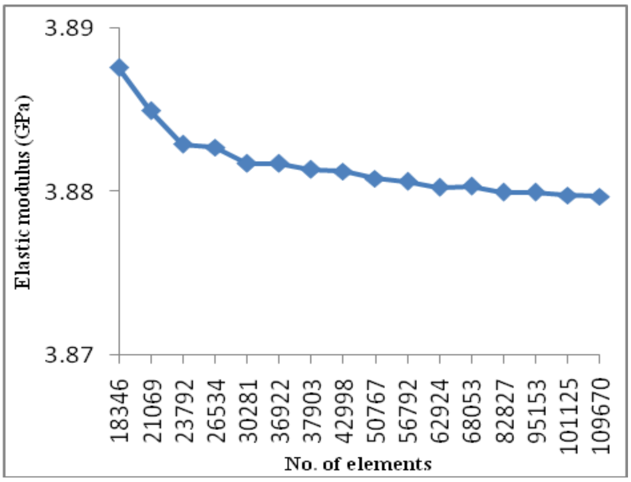

Figure 4: Variation of elastic modulus with no. of element for 1% volume fraction of alumina particles

2.3 Convergence test

Convergence test was performed for RVE of size 325nm with 1% volume fraction of alumina particles to determine correct size of element for analysis. Elastic modulus was evaluated by varying the element size. Number of elements corresponding element size is in **Table 1**.

It is clear from **Fig 4** that by increasing the number of elements from 18346 to 109670, there is decrease in elastic modulus. Elastic modulus of composite does not change much (0.05%) if the number of elements is increased beyond 30281. So, the element size (35nm) corresponding to 30281 number of element can be taken.

2.4 Halpin-Tsai model

The results obtained from finite element analysis were compared with that obtained from Halpin-Tsai analytical model. Halpin-Tsai equation for elastic modulus of composite of short fiber is given by **[7]**

$$E = \frac{E_m(1 + \eta\xi V_f)}{(1 + \eta\xi)}$$

$$Where \quad \eta = \frac{E_f/E_m - 1}{E_f/E_m + \xi}$$

$$and \quad \xi = 2 + 40V_f^{10} \quad for\ spherical\ shape\ reinforcement$$ [19]

Where E_f and E_m are the elastic modulus of fiber and matrix respectively, V_f is volume fraction of fiber, ξ is shape parameter depending upon filler geometry and loading direction.

3 Results and Discussion

3.1 RVE sizing

The size of RVE should be such that the RVE should contain adequate number of particles to provide a statistically equivalent representation of the composite. To obtain the correct size of RVE, analysis was carried out for composite having 1% volume fraction of alumina particle. Number of particles required for various size of RVE is given in Table 2. Composite having 1% volume fraction of particles was considered for the analysis because the distance between adjacent particles will be the larger for lower percentage of reinforcement. For each size of RVE, elastic modulus was evaluated for three different configurations of randomly distributed particles. For any one of three configurations, elastic modulus was evaluated in all x, y, z directions. The average elastic modulus of composite as a function of particle is plotted in the **Fig 5**. It is clear from **Fig. 5** that the elastic modulus decreases as the RVE size increases. But the change in elastic modulus is very less (0.1%) when RVE size increased from 260nm to 470nm. The change in the elastic modulus was in the range of standard deviation of that analysis. So, RVE size of 260nm was considered for finite element analysis in the present work. The L/D ratio (L=260nm, D=40nm) for RVE considered in this work is 6.5,

Table 1 Variation of no. of element with element size in RVE for 1% volume fraction of alumina

Element size(nm)	85	55	45	40	35	31	29	27	25	23	21	20	18	17	16
No. of elements	18346	21069	23792	26534	30281	36922	37903	42998	50767	56792	62924	68053	82827	95153	101125

which is in confirmation with the earlier reported work **[15].** Number of particles were increased for composite having higher volume fraction of alumina particles.

Table 2 variation of number of spherical particles with RVE size for 1% volume fraction of nanocomposite

RVE Size (nm)	260	350	370	410	440	470
No. of spheres	5	10	15	20	25	30

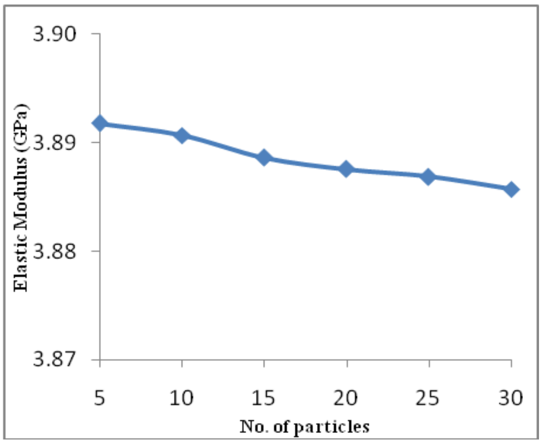

Figure 5: Variation of elastic modulus as a function of no. of alumina particles (RVE size) for composite having 1% volume fraction of alumina particles

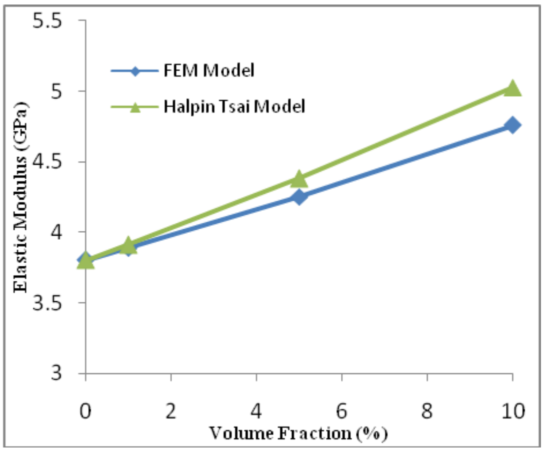

Figure 6: Variation of elastic modulus as a function of volume fraction of alumina particle

Total five configurations of RVE have been analyzed for each volume fraction and the average elastic modulus, standard deviation and 95% confidence level are given in table in **Table 3**. Elastic modulus of composite as a function of particle volume fraction is given in **Fig. 6.** An increment of 26% in the elastic modulus of composite having 10% volume fraction alumina particle over that of neat epoxy was evaluated whereas Halpin-Tsai equation gives an increment of 32% for composite having 10% of volume fraction of spherical shape particles.

Conclusion

In this paper we have focused on the evaluation of effective material properties of nanocomposite of epoxy reinforced with randomly distributed spherical shape Al_2O_3 particles of 40nm diameter using finite element based RVE with symmetric boundary conditions. Elastic modulus evaluated by finite element modeling exhibits good agreement with Halpin-Tsai analytical model at low volume fraction. Elastic modulus is evaluated up to 10% volume fraction of alumina particles.

References

1. Reuss A. “Berechnung der Fliessgrenze von Mischkristallen auf Grund der Plastizitatsbedingung fur Einkristalle” Journal of applied Math Mech 9 (1929) 49–58.
2. Voigt, W. "Theoretische Studien über die Elasticitätsverhältnisse der Krystalle".*Abh.Kgl.Ges.Wiss.Göttingen, Math.Kl.* 34 (1887) 3–51.
3. Hashin Z. “The elastic moduli of heterogeneous materials” J Appl Mech 29 (1962) 143–150.
4. Eshelby JD.” The determination of the elastic field of an ellipsoidal inclusion and related problems” Proc Roy Soc A 241 (1957) 376–396
5. Mori T, Tanaka K. “Average stress in the matrix and average elastic energy of materials with misfitting inclusions”. Acta Metall Mater 21 (1973) 571–574.
6. Benveniste Y. “A new approach to the application of Mori–Tanaka theory in composite materials”. Mech Mater 6 (1987) 147–157.
7. J.C. Halpin, J.L. Kardos, “The HalpinTsai equation: a review” Polymer Engineering and Science 16 (1976) 344–352.
8. Jyi-Jiin Luo, Isaac M. Daniel, “Characterization and modeling of mechanical behavior of polymer/clay nanocomposites”Composites Science & Technology63(2003)1607–1616
9. Bernd Wetzel, Patrick Rosso, Frank Haupert, Klaus Friedrich,” Epoxy nanocomposites – fracture and toughening mechanisms” Engineering Fracture Mechanics 73 (2006) 2375–2398

Table 3 variation of elastic modulus with volume

Voume Fraction (%)	FEM Model E (GPa)	% increased Elastic Modulus	Standard Deviation	Confidence Level	Halpin-Tsai Model E (GPa)	% increased Elastic Modulus
0	3.8	0	0	0	3.8	0
1	3.89	2.35	0.0024	0.0021	3.91	2.894736842
5	4.25	11.7	0.00832	0.0073	4.38	15.26315789
10	4.758	25.21	0.0138	0.0121	5.02	32.10526316

10. Suraj C. Zunjarrao, Raman P. Singh, “Characterization of the fracture behavior of epoxy reinforced with nanometer and micrometer sized aluminum particles” Composites Science and Technology 66 (2006) 2296–2305
11. Tadaharu Adachi, Mayuka Osaki, Wakako Araki, Soon-Chul Kwon, “Fracture toughness of nano- and micro-spherical silica-particle-filled epoxy composites” Acta Materialia 56 (2008) 2101–2109
12. Dharmendra Kumar Shukla , Venkitanarayanan Parameswaran,” Epoxy composites with 200 nm thick alumina platelets as reinforcements” J Mater Sci 42(2007) 5964–5972
13. Dharmendra Kumar Shukla, Subramanyam V. Kasisomayajula, Venkitanarayanan Parameswaran, “Epoxy composites using functionalized alumina platelets as reinforcements” Composites Science and Technology 68 (2008) 3055–3063
14. Prabhakar R. Marur, “Estimation of effective elastic properties and interface stress concentrations in particulate composites by unit cell methods” Acta Materialia 52 (2004) 1263–1270
15. Sreedhar Kari , Harald Berger , Reinaldo Rodriguez-Ramos , Ulrich Gabbert, “Computational evaluation of effective material properties of composites reinforced by randomly distributed spherical particles” Composite Structures 77 (2007) 223–231
16. K. Hbaieb, Q.X. Wang , Y.H.J. Chia, B. Cotterell, “Modeling stiffness of polymer/clay nanocomposites” Polymer 48 (2007) 901e909
17. Venkitanarayanan Parameswaran, Dharmendra Kumar Shukla, “Evaluation of elastic modulus of epoxy reinforced with 200nm thick alumina platelets through finite element analysis” Material Science and Engineering A 527 (2010) 3792-3799
18. S. Nemat-Nasser, M. Hori, Micromechanics: Overall Properties of Heterogeneous Materials, Elsevier, Oxford, 1999.
19. P.K. Mallick, “Fiber Reinforced Composite”
20. H.W. Wanga, H.W. Zhou , R.D. Peng, Leon Mishnaevsky Jr. ”Nanoreinforced polymer composites: 3D FEM modeling with effective interface concept” Composites Science and Technology 71 (2011) 980–988
21. A. Alavinasab, R. Jha , G. Ahmadi, C. Cetinkaya, I. Sokolov “Computational modeling of nano-structured glass fibers” Computational Materials Science 44 (2008) 622–62
22. Behnam Ashrafi, Pascal Hubert”Modeling the elastic properties of carbon nanotube array/polymer composites” Composites Science and Technology 66 (2006) 387–396
23. E. Shady, Y. Gowayed “Effect of nanotube geometry on the elastic properties of nanocomposites” Composites Science and Technology 70 (2010) 1476–1481
24. G.M. Odegarda, T.C. Clancy, T.S. Gates “Modeling of the mechanical properties of nanoparticle/polymer composites” Polymer 46 (2005) 553–562
25. N. Chawla, V.V. Ganesh, B. Wunsch ”Three-dimensional (3D) microstructure visualization and finite element modeling of the mechanical behavior of SiC particle reinforced aluminum composites“ Scripta Materialia 51 (2004) 161–165
26. S. Malinov, W. Sha “Software products for modelling and simulation in materials science” Computational Materials Science 28 (2003) 179–198
27. K. Anoukou, F. Zaïri, M. Naït-Abdelaziz, A. Zaoui , T. Messager , J.M. Gloaguen “On the overall elastic moduli of polymer–clay nanocomposite materials using a self-consistent approach. Part I: Theory” Composites Science and Technology 71 (2011) 197–205
28. K. Anoukou, F. Zaïri, M. Naït-Abdelaziz, A. Zaoui , T. Messager , J.M. Gloaguen “On the overall elastic moduli of polymer–clay nanocomposite materials using a self-consistent approach. Part II: Experimental varification” Composites Science and Technology 71 (2011) 206–215
29. C. Pisano , P. Priolo, Ł. Figiel, “Prediction of strength in intercalated epoxy–clay nanocomposites via finite element modelling” Computational Materials Science 55 (2012) 10–16