Theoretical Predictions on Mechanical Properties of Functionally Graded Epoxy/Clay Nanocomposites

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Abstract: In this paper, the theoretical predictions of mechanical properties of functionally graded and uniform distributions Epoxy/clay nanocomposites are presented. The specimens were prepared for uniformly distribution of nanoclay with different nano particles weight percent (pure, 3 wt%, 5 wt% and 7 wt%) and functionally graded distribution. The distribution of nanoparticles has been investigated by Field Emission Scanning Electron Microscopy (FESEM). For uniformly distribution of nanoclay, it is shown that there is no sign of the agglomerates found via FESEM imaging which can address well the distribution of nanoclay particles in epoxy. In addition, for functionally graded distributions, it is found that dispersion of nanoclays vary smoothly and continuously from one surface to the other one. The mechanical properties have been determined by simple extension tests. The results of extension tests show that elastic modulus begins to increase up to 5 wt% of nanoclay and then decreases. So, for functionally graded distribution, the elastic modulus is generally larger than the corresponding values for uniform distribution of nanoclay. The theoretical predictions of Young's modulus for functionally graded and uniform distributions nanocomposites are calculated using a genetic algorithm procedure. The formulation for Young modulus includes the effect of nanoparticles weight fractions and it is modified for functionally graded distribution. To investigate the accuracy of the present theoretical predictions, a comparison is carried out with the experimental results. It is found that the results obtained from the theoretical predictions of genetic algorithm procedure are in good agreement with the experimental ones.

Keywords: Epoxy, Clay, Functionally Graded, Genetic Algorithm Theory, Nanoparticles

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Biographical notes: Mahdi Karami Khorramabadi received his PhD in Mechanical Engineering from Razi University in 2018. He is currently Assistant Professor at the Department of Mechanical Engineering, Islamic Azad University, Khorramabad Branch, Lorestan, Iran. He has published more than 34 papers in various refereed national and international journals and conferences. His current research interest includes preparation of functionally graded nanocomposites and modelling with theoretical predictions on mechanical properties of polymer/clay nanocomposites. His research also focuses on theoretical, experimental and numerical analysis of mechanical buckling, free and forced vibration and dynamic stability of functionally graded and uniform distribution nanocomposite beams, plates and shells.

1 INTRODUCTION

During the last decades, the application of composite materials in various structures has become increasingly popular, especially in aerospace structures, ship hulls and airframes. Composites are preferred above conventional materials because of their advantages such as high specific strength and stiffness. In this manner, epoxy resins, as matrix part, are widely applied to various engineering fields due to their excellent mechanical and insulation properties. These resins are reinforced with various particles or fibers to improve their properties further. The particle size is currently being decreased to below the micrometer level to form nano composites with better mechanical properties. The reinforcement part can be either particle such as nanoclay or tube such as carbon nanotubes or platelet like nanoclay. In the following, some recent works have been listed.

The interest in clay-polymer nanocomposites has increased ever since Toyota demonstrated commercial applications of nylon 6/clay nanocomposites [1]. Other types of nanoparticles are also being incorporated into polymeric resins in order to fabricate materials with increased performance. The nanoscale particles possess enormous surface area. Hence, the interfacial area between the two intermixed phases in nanocomposite is substantially larger than traditional composites. This results in increased bonding between the particles and the matrix. Therefore, several mechanical, thermal and electrical properties of nanocomposites are observed to be better than those of conventional microcomposites or the neat matrix resin [2–9]. Mortazavi et al. [10] investigated the effect of addition of nanosilica to pure epoxy and found that the elastic modulus increases. This is maybe due to strong bondings between matrix and nanoparticles.

Wang et al. [11] found that by addition of nanosilica to pure epoxy, the Young’s modulus and tensile strength increase. In another study, Wang et al. [12] showed that by addition of nanosilica to cyanate resin, the tensile strength and toughness increase. Meybodi et al. [13] investigated a new approach for prediction of elastic modulus of polymer/nanoclay composites by considering interfacial debonding. They used the experimental and numerical methods to investigate the elastic modulus of polymers reinforced with nanoclay. In another study, Meybodi et al. [14] found that the effect of nanoparticles on energy absorption is more considerable at higher impact energies. Ayatollahi et al. [15] showed that the multi-walled carbon nanotubes and nanosilica enhanced the fiber–matrix interfacial strength and then by toughening the surrounding matrix, improved the strength and stiffness of multi-scale composites. Goodarz et al. [16] studied the quasi-static indentation of aramid fiber/epoxy composites containing naylon 66 electrospun nano-interlayers. Monfared et al. [17] indicated that by adding the hybrid nanoparticles to the unfilled carbon fabric composites, the friction coefficient variation of these specimens totally changed, which led to an improvement in the friction-reducing ability and wear rate resistance. Maghsoudlou et al. [17] found that the simplest cylindrical representative volume element has the greatest discrepancy with experimental results which showed the necessity of consideration of three important parameters including single-walled carbon nanotubes interphase, curvature, and agglomerations.

Based on the previous literature studies, it appears that the preparation and mechanical properties of uniformly distributed epoxy/ clay nanocomposite have been extensively investigated. However, there is no report on the theoretical predictions of mechanical properties of functionally graded Epoxy/Clay nanocomposites in the open literature. The present study deals with the theoretical predictions of mechanical properties of functionally graded Epoxy/Clay nanocomposites. The distribution of nanoparticles has been investigated by Field Emission Scanning Electron Microscopy (FESEM). By using the genetic algorithm procedure, Young’s modulus of nanocomposites for functionally graded and uniform distribution is calculated and then is compared with the experimental results. It is found that the results obtained from the genetic algorithm approach are in good agreement with the experimental ones.

2 EXPERIMENTAL PROCEDURE

2.1. Materials

The polymer matrix used in this study was an Epoxy with trade name PR7000 from AL TANNA Co. (Germany), with density $\rho = 2.25 g/ml$. The hardener was mixed in the ratio of 10:1. The nanofiller was US7810 from US Research Nanomaterials Inc., USA.

2.2. Nanocomposite Fabrication

2.2.1. Uniform distribution (UD)

The nanoclay was firstly dried at 40^0c in a vacuum oven for a minimum of 48 hrs and introduced into the epoxy resin and mixed well with a glass rod before subjected to mechanical stirring at 500 rpm for 1 hr. Secondly, the clay–resin mixture was poured out into a beaker and heated up in a hot water bath at 50^0c to lower down the viscosity. Then, the mixture was treated with ultrasound for 20 min. Ultrasonic stirring from Hielscher, Germany (model UP400S) were used to ultrasound. After that the mixture was cooled down, the appropriate amount of hardener according to the above said mixing ratio was added and mixed well. For degas the mixture, vacuum chamber from HBS, China (model HBS-3C) is applied for 30 min. Finally, the whole mixture was poured inside a dumbbell-shape mould for curing and forming. The full curing of samples was done by leaving it for a day at the room temperature and then curing at 120 °C for 2 hr. The preparation procedure for uniform distribution is presented in “Fig. 1”.

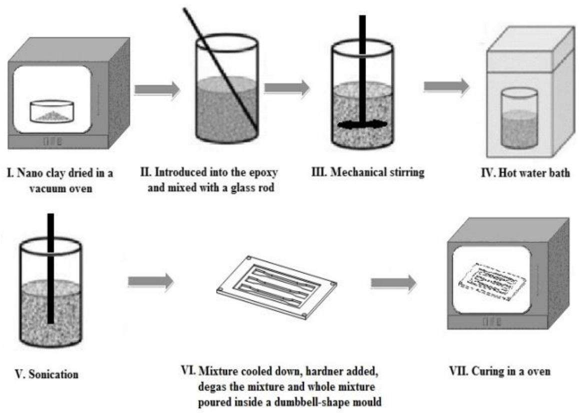

Fig. 1 Preparation procedure for uniform distribution.

2.2.2. Functionally Graded Distribution (FGD)

For functionally graded distribution, the preparation procedure for uniform distribution was done for samples with 1 mm thicknesses. The thickness of each sheet is 1 mm and four sheets with different nano particles weight percent (pure, 3 wt%, 5 wt% and 7 wt%) were employed to make functionally graded nanocomposite. In order to provide good adhesion between sheets, epoxy can be used as adhesive film. The products were compressed and then moulded into sheets by an electrically heated hydraulic press. The preparation procedure for functionally graded distribution is presented in “Fig. 2”.

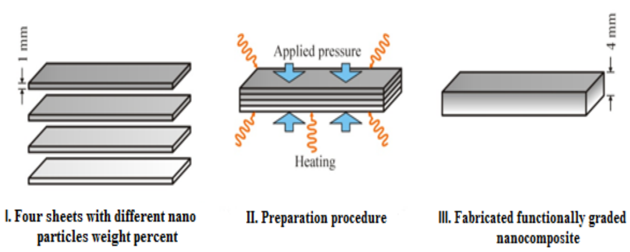

Fig. 2 Preparation procedure for functionally graded distribution.

2.3. Morphology

To investigate the morphology of nanocomposites samples, Field Emission Scanning Electron Microscope (FESEM) pictures were taken at Lorestan University. The morphology of nanocomposites cross section samples for uniform and functionally graded distributions were observed by a TESCAN MRIA3 Field Emission Scanning Electron Microscope (FESEM) after sputter coated with gold. Figure 3 is the FESEM photography of nanocomposite for uniform distribution and “Fig. 4” is the FESEM photography of nanocomposite for functionally graded distribution.

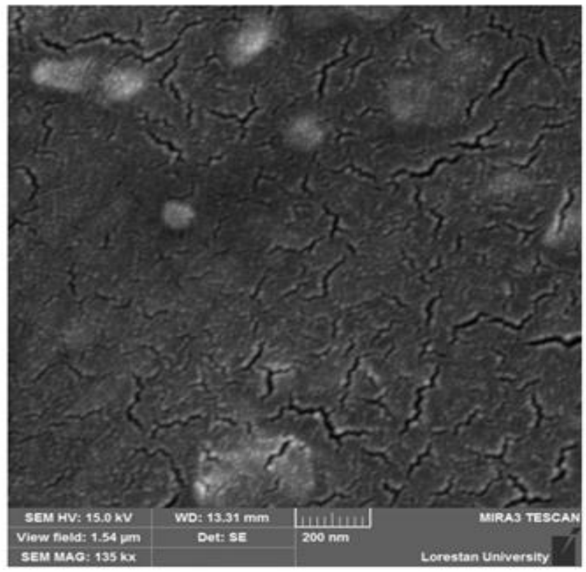

Fig. 3 FESEM image of nanocomposite for uniform distribution.

The FESEM photography of epoxy-nanoclay composite at 3 wt% has been shown in “Fig. 3”. There is no sign of the agglomerates found via FESEM imaging which can address well the distribution of nanoclay particles in epoxy at 3 wt% specimens which is maybe due to well sonication by ultrasonic probe. Moreover, “Fig. 3” demonstrates the peeled section which is maybe due to propagation of crack across the boundary which is weaker compared to other parts of the material.

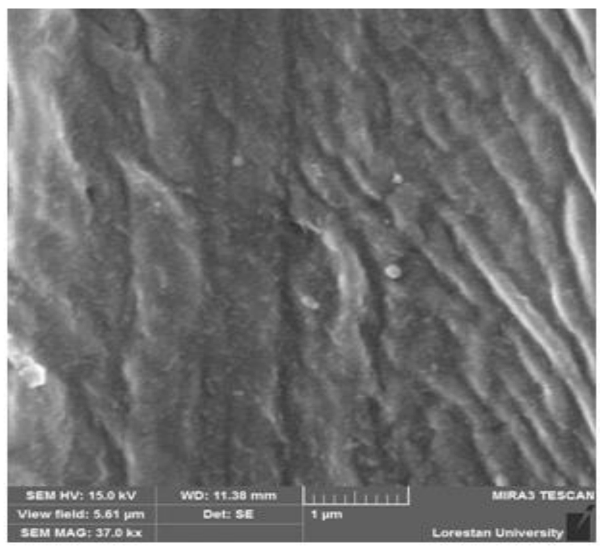

Fig. 4 FESEM image of nanocomposite for functionally graded distribution.

Figure 4 shows that the interface of the layers has melted, the layers at the interfaces completely are mixed and no distinct interface can be detected. In addition, there is no sign of the agglomerates which were found. Therefore, the dispersion of nanoclays vary smoothly and continuously from one surface to the other one.

2.4. Mechanical Properties

The specimens were tested according to ASTM D638 with three repeats. The tension tests were carried out using Gotech universal testing machine (Model GT-AI5000L) with a crosshead speed of 50 mm/min as shown in "Fig. 5".

Fig. 5 The Gotech universal testing machine (Model GT-AI5000L).

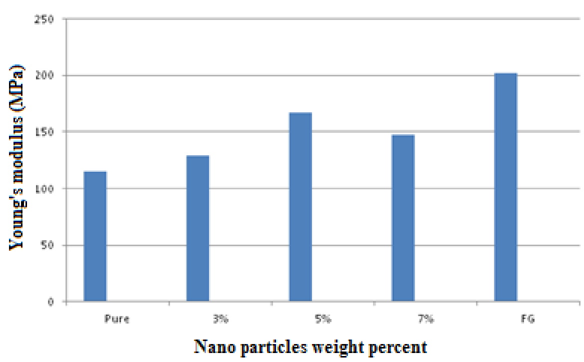

Fig. 6 The Young's modulus of nanocomposites with different distribution of nano particles.

Tensile tests are used to determine how nanocomposite will behave under tension load. In a simple tensile test, a sample is typically pulled to its breaking point to determine the mechanical properties of the nanocomposite. The amount of tensile force applied to the sample and the displacement of the sample are measured throughout the test. As they pull sample apart, Gotech testing machines accurately calculate the tensile modulus. The values of the nanocomposites Young's modulus for functionally graded and uniform distribution of nanoclay are shown in "Fig. 6".

It is shown that elastic modulus begins to increase up to 5 wt% of nanoclay and then decreases. So, for functionally graded distribution, the elastic modulus is generally larger than the corresponding values for uniform distribution of nanoclay. The agglomeration of nan clay particles on 7 wt% percentage of nanoclay in epoxy/ nano clay nanocomposite can be seen where this effect verifies the decrement of elastic modulus compared with other specimens.

3 MATHEMATICAL MODELING

In computer science and operations research, a Genetic Algorithm (GA) is a metaheuristic inspired by the process of natural selection that belongs to the larger class of Evolutionary Algorithms (EA). Genetic algorithms are commonly used to generate high-quality solutions to optimization and search problems by relying on bio-inspired operators such as mutation, crossover and selection. The GA method searches for the best alternative (in the sense of a given fitness function) through chromosome evolution [19]. The basic steps in the GA analysis are shown in "Fig. 7".

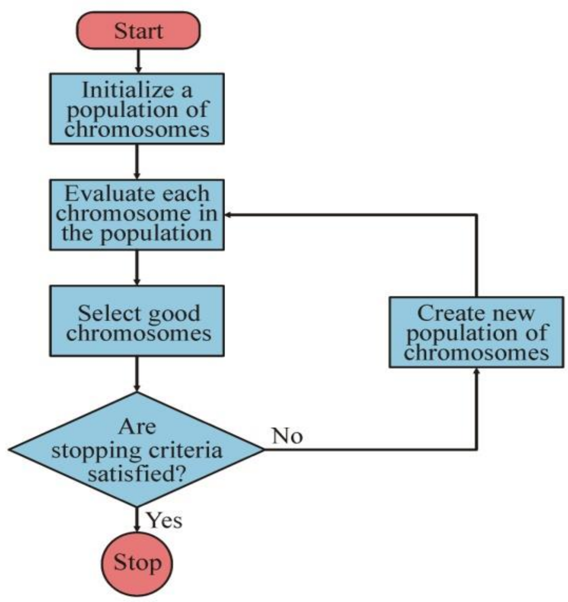

Fig. 7 High-level description of the GA.

As shown above, at first an initial population of chromosomes is randomly selected. Then each of the chromosomes in the population is evaluated in terms of its fitness (expressed by the fitness function). Next, a new population of chromosomes is selected from the given population by giving a greater chance to select chromosomes with higher fitness. This is called the reproduction operation. The new population may contain duplicates. If given stopping criteria (e.g., no chance in the old and new population, specified computing time, etc.) are not met, some specific, genetic-like operations are performed on chromosomes of the new population. These operations produce new chromosomes, called offspring. The same steps of this process, evaluation and reproduction operation are then applied to chromosomes of the resulting population. The whole process is repeated until the given stopping criteria are met. The solution is expressed by the best chromosome in the final population. In this paper, the "$1 - R^2_{adj}$" is introduced as the fitness function which is to be minimized. "R^2_{adj}" is the accuracy criterion of an arbitrary mechanical property function (such as Young's modulus). "R^2_{adj}" is defined as a process which is demonstrated below. The mechanical property is function of nanoclay weight percent and "R^2_{adj}" is a function of coefficients which are introduced below. M_i is considered as the mechanical properties and "W" as the nano clay weight percent.The M_i is expressed as a polynomial function of "W" as follows:

$$M_i = \sum_{j=0}^{4} a_{ji} W^j \tag{1}$$

Now, the coefficients a_{ji} are found by maximizing the accuracy of polynomial function. The equations can be written as:

$$R^2_{adj} = 1 - \frac{VAR_E}{VAR_T} \tag{2}$$

In which

$$VAR_E = SS_{Err}/(n-k-1) \tag{3}$$

$$VAR_T = SS_{Tot}/(n-1) \tag{4}$$

$$SS_{Tot} = \sum_{i=1}^{n} (y_i - \bar{y})^2 \tag{5}$$

$$SS_{Err} = \sum_{i=1}^{n} (y_i - M_i)^2 \tag{6}$$

$$\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i \tag{7}$$

$$M_i(W) = a_{0i} + a_{1i} W + a_{2i} W^2 + a_{3i} W^3 \tag{8}$$

In these equations, $n = 4$ is the number of experiments and $k = 0$ is the number of duplicated experiments and y_i shows the experimentally measured mechanical properties. After minimization of "$1 - R^2_{adj}$" via MATLAB, factors a_{ji} are obtained after approximately 40 generations. Obtaining the a_{ji} coefficients, the Young's modulus can be expressed as functions of nanoclay weight percent as follows:

$$E = -25.145w + 14.276w^2 - 1.432w^3 + 115.108 \tag{9}$$

Here, w is the nanoclay weight percent. "Eq. (9)" can be used to derive the suitable relation for Young's modulus of functionally graded distribution. The specimen with functionally graded distribution consists of four perfectly bonded sheets with a total thickness of 4 mm. Each sheet has 1 mm thickness with different nanoparticles weight fractions (pure, 3 wt.%, 5 wt.% and 7 wt %). The Young's modulus can be written as:

$$\begin{aligned} E(z) = {} & -25.145(2[z] + Sgn[z]) + 14.276(2[z] + Sgn[z])^2 \\ & -1.432(2[z] + Sgn[z])^3 + 115.108 \end{aligned} \tag{10}$$

4 RESULTS AND DISCUSSION

The results of mechanical tests and theoretical predictions for the Young's modulus of uniform distribution nanocomposites are presented in "Table 1".

Table 1 Comparison of Young's modulus for uniform distribution nanocomposites

Nanoclay weight percent	Theoretical predictions (Mpa)	Experimental Results (Mpa)
pure	115.108	115.108
3%	129.493	129.486
5%	167.283	167.258
7%	147.441	147.379

The compression between theoretical predictions and the experimental data shows the high accuracy of the present analysis. The results of mechanical test cannot be employed to investigate the correctness of theoretical prediction for functionally graded distribution nanocomposite. Thus, to investigate the accuracy of theoretical prediction for functionally graded distribution nanocomposite, the static analysis was employed. As mentioned before, the Young's modulus is assumed to vary as a function of the thickness coordinate $z(0 \le z \le 4)$.

"Eq. (10)" can be verified via employing the static analysis of functionally graded nanocomposite beam under transverse load. It is considered as a functionally graded nanocomposite beam as shown in "Fig. 8".

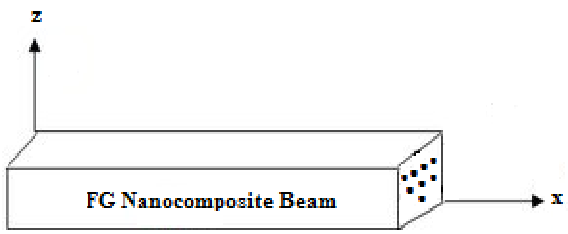

Fig. 8 Schematic of the problem studied.

The thickness, length, and width of the beam are denoted, respectively, by h, L and b. The position of neutral surface can be determined as [20]:

$$h_0 = \frac{\int_{-\frac{h}{2}}^{\frac{h}{2}} E(z) z dz}{\int_{-\frac{h}{2}}^{\frac{h}{2}} E(z) dz} \tag{11}$$

For Euler-Bernoulli theory, differential equation of deflection can be expressed as [20]:

$$\frac{d^2 w}{dx^2} = \frac{M(x)}{D} \tag{12}$$

Where D denotes bending rigidity of the FG nanocomposite beam defined by [20]:

$$D = \int_{-\frac{h}{2}}^{\frac{h}{2}} bE(z)(z - h_0)^2 dz \tag{13}$$

Boundary conditions for simply supported beam are:

$$w = \frac{d^2 w}{dx^2} = 0 \quad \text{at} \quad x = 0 \quad \text{and} \quad x = L \tag{14}$$

By integrating "Eq. (12)" and then applying the boundary conditions ("Eq. 14"), one can easily obtain the deflection of the beam under the transverse load. For experimental static analysis of functionally graded nanocomposite beam under transverse load, the beam apparatus from TQ, England (Model SM1004) was used for deflection test as shown in "Fig. 9".

The test specimen has a rectangular cross section $20 \times 4\ mm^2$ and a length of $15 cm$ and the load magnitude is $0.54N$. The comparison between theoretical and experimental data of deflection for functionally graded distribution nanocomposites is shown in "Table 2".

Fig. 9 The beam apparatus TQ (Model SM1004).

Table 2 Compression between theoretical and the experimental data of deflection

Boundary condition	Load position- x (cm)	Deflection measuring position-x (cm)	Theoretical deflection (mm)	Experimental deflection (mm)
simply support	5.5	7.5	2.54	2.43

It is shown that the presented approach for modelling of Young's modulus of functionally graded distribution nanocomposites has high accuracy.

5 CONCLUSIONS

In this paper, theoretical prediction on mechanical properties of functionally graded epoxy/clay nanocomposites was investigated. By addition nanoclay particles, the elastic modulus begins to increase up to 5 wt% of nano clay. This is maybe due to the existence of strong and sufficient bonding between epoxy and nanoclay particles. The agglomeration of nanoclay particles is maybe due to decrease of the elastic modulus for 7 wt% of nanoclay. In other words, these particles are changed to stress concentration sites and positions for crack propagation. Moreover, for functionally graded distribution, the elastic modulus is generally larger than the corresponding values for uniform distribution of nanoclay. The comparison between theoretical predictions and the experimental data for elastic modulus of uniform and functionally graded distributions shows the high accuracy of genetic algorithm procedure.

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