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Investigating the effects of number and distribution of GNP layers on graphene reinforced polymer properties: Physical, numerical and micromechanical methods

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ABSTRACT

Experimental, numerical and micromechanical methods have been used to determine mechanical properties of graphene nanoplatelets (GNPs) reinforced epoxy resin. Tensile and compressive tests were performed on samples containing different GNP weight fractions. Experimental measurements showed an improvement in epoxy resin tensile and compressive mechanical properties with increasing GNP weight fraction. Also, Field Emission Scanning Electron Microscope (FESEM) was used to obtain images of the samples' fracture surfaces. These images suggested a good GNP dispersion in the matrix. Numerical simulations were carried out to investigate the effects of different geometrical parameters such as: number of GNP layers, GNP orientation, GNP distribution, and GNP/matrix interface on nanocomposite mechanical properties. Three different models containing one, two, and three layers of GNPs were analyzed to investigate the effects of number of GNP layers on nanocomposite properties. The GNP/matrix interface was modeled using several thin layers with different stiffness values surrounding the GNPs. The results of this investigation suggest that nanocomposite longitudinal modulus decreases with increasing the number of graphene layers. Also, the model consisting two layers of GNPs predicts values closer to experimental results. In addition, models consisting of GNPs oriented at different spatial orientations were analyzed to investigate the effect of GNP orientation on nanocomposite mechanical properties. It was observed that, GNP orientation significantly affects the nanocomposites elastic modulus. Moreover, Halpin-Tsai micromechanical model was used to estimate the nonlinear tensile stress-strain behavior of nanocomposites for randomly-distributed GNP nanocomposites. Finally, numerical and micromechanical results were compared and excellent correlation with experimental measurements was observed.

1. Introduction

Although, the addition of carbon nanotubes or nanofibers into thermosetting resins can improve their mechanical, thermal and electrical properties, the industrial application of these materials is generally limited by two main factors. These limiting factors are the poor dispersion of nanofibers, which implies the need for complex procedures to achieve good dispersion [1–3], and the high cost of carbon nanotube synthesis [2]. Both of these limitations cause an excessive price increase, which is not compensated by the enhancement of properties on numerous occasions. Recently, graphene due to its high aspect ratio (few-atoms thick), high specific surface area, strong sp^2 carbon–carbon bonds, and low cost compared to carbon nanotubes has attracted much attention for use as a reinforcement material in nanocomposites [1–5].

Many researchers have experimentally determined mechanical and physical properties of epoxy based nanocomposites containing various Graphene Nanoplatelet (GNP) weight fractions under different loading conditions [6–11]. The results indicate significant improvement in mechanical properties, thermal conductivity, fracture toughness and fatigue behavior of nanocomposites [6–10]. Also, it was observed that strain rate plays a more noticeable role under compressive loading in comparison to tensile loading for these nanocomposites [11]. In addition, combinations of sonication and reinforcement chemical modification have been used to

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improve nanocomposite mechanical properties [12–14]. It is found that chemical modification and functionalization of graphene are effective in improving their dispersion stability and inhibit their re-agglomeration during the curing of resin. In fact, improvements in nanocomposite mechanical properties have been reported when sonication process is used [13,14]. Also, the effect of graphene nanoplatelets' orientation on nanocomposite Young's modulus was investigated [15]. It was observed that, random orientation of graphene reduces nanocomposite Young's modulus by almost a factor of 2 compared with the fully-aligned reinforcement case. In addition, hybrid nanocomposites have been prepared with different methods such as growing carbon nanotubes on GNPs and using this hybrid reinforcement in epoxy matrix [16]. Micro-mechanical, molecular dynamics, and finite element approaches have been used in recent years to estimate nanocomposite mechanical properties [17–21]. The results of these investigations show good correlations between predicted and experimentally determined elastic moduli.

According to the presented literature review, many researchers have determined mechanical properties of GNP reinforced polymers using experimental, numerical and micromechanical methods in recent years. However, these investigations have been limited to the determination of elastic modulus of nanocomposites under tensile loading conditions. Nonlinear tensile mechanical behavior of GNP nanocomposites has not been investigated using micromechanical methods. Also, mechanical properties of randomly distributed GNP reinforced epoxy have not been determined numerically. In this investigation, tensile and compressive mechanical properties of GNP-reinforced epoxy with various weight fractions have been determined using experimental, numerical and micromechanical methods. For this purpose, standard nanocomposite samples were prepared and were subjected to tensile and compressive loadings. Also, Field Emission Scanning Electron Microscope (FESEM) was used to obtain images of the specimen's fracture surfaces and to assess GNP dispersion in the matrix. In addition, numerical simulations of nanocomposites were conducted in ABAQUS finite element software. In these simulations, the effects of various geometrical parameters such as: the number of GNP layers, orientation, and distribution on nanocomposite modulus of elasticity were investigated. For this purpose, models consisting of one, two and three layers of GNP were analyzed to investigate the effect of number of GNP layers. A smooth strength transfer between the GNP and matrix was created by using eleven thin layers of elastic material. In addition, GNP layers were rotated about two axes to investigate the effects of GNP orientation on nanocomposite properties. Also, randomly distributed GNP reinforced epoxy was modeled as a more realistic nanocomposite. Moreover, tensile stress-strain behavior of nanocomposites was predicted using Halpin-Tsai micromechanical model. Finally, experimental, numerical, and micromechanical results were compared and good agreement was observed.

2. Experimental

2.1. Materials

In this research, Manapar R510, based on bisphenol-A polymeric resin and Manapar H520 as a corresponding hardener was used as the matrix material with 100:20 mix ratio by weight. GNPs used as the reinforcements were obtained from US Research Nanomaterials Inc. (US-NANO). Specifications of reinforcement are listed in Table 1.

2.2. Specimen preparation

Tensile and compression test specimens were prepared by adding the desired amount of GNPs (i.e. 0, 0.25, 0.5, 0.75, and 1.0 wt %) to the monomer. To decrease initial viscosity of epoxy, pre-heating was applied to the solution. Next, this mixture was stirred using a mechanical stirrer at a speed of 1000 rpm for 90 min. In order to homogenize the dispersion and to break the GNP agglomeration, the mixture was sonicated for 30–60 min based on reinforcement weight fraction. For this purpose, an ultrasonic homogenizer was used set at 200 W power and 24 Hz frequency. Iced water bath was used to keep down the temperature of the solution during the sonication process. The sonication process was paused for 30 s after every 2 min of sonication. Next, the solution was placed under vacuum for 15 min to remove any trapped air. After degassing, the hardener was added and the solution was stirred gently for 10 min. Then, this solution was placed under vacuum for 10 min again. Finally, the nanocomposite solution was poured into a steel mold and was cured at 25 °C for 16 h followed by a two-hour post cure at 100 °C.

Table 1
GNP specifications.

Young modulus	Diameter	Thickness	Number of layers	Purity
1000 *GPa*	$4-12\ \mu m$	$2-18(nm)$	Less than 32 Layers	99.5%

2.3. Characterization

Tensile and compressive mechanical properties of pure resin and nanocomposites were determined by performing tensile and compressive tests on several samples at each GNP weight fraction. Tensile and compressive specimens were prepared and were tested according to D638-IV and D695 ASTM standards, respectively [22,23]. A picture of the standard specimens with 1.0 wt % GNPs is shown in Fig. 1. Four tensile test specimens with dimensions 115 mm long × 12.7 mm wide and 3 mm thick in a dog-bone shape were prepared and were tested at each GNP weight fraction. Also, four 9 mm long with 8.5 mm diameter cylindrical compression test specimens were prepared and were tested at each GNP weight fraction. Thus, a total of 40 tests were conducted. Santam universal testing machine STM-20 with a 20 kN load cell was used to perform these tests. Tensile and compression tests were performed at a speed of 10 mm/min and 0.5 mm/min, respectively [24].

Also, Fourier Transform Infrared Spectroscopy (FTIR) model Tensor 27 powered by ATR system was used to investigate the surface properties of pure epoxy, GNP, and nanocomposite. The spectra were recorded between 4000 and 600 cm^{-1} frequency ranges.

2.4. SEM and FESEM image analysis

SEM and FESEM images were obtained from fracture surfaces of

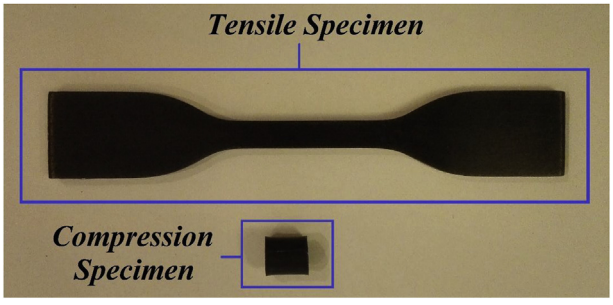

Fig. 1. Nanocomposite standard tensile and compression specimens containing 1.0 wt % GNPs.