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Structural and Viscoelastic Characteristics of Numerous Layered Graphene/Epoxy Nanocomposites

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ABSTRACT

One atom - thick planar, covalently bonded to three other atoms in a tightly populated, two-dimensional (2D), hexagonal single layer stable crystal hexagonal lattice, graphene is a flattened monolayer of carbon atoms. This study describes the production of in-situ amine placed in contact gently exfoliate graphene with many layers, low degradation contents, and average aspect ratios up to 10 micron and thickness up to 2-3 Nano meter. For this study, we developed Found that participants composites (AF-MGL/EpC) with graphene fractions between 0.5 and 2.0 wt percent. The graphene concentrations used to create the four separate samples were 0.0, 0.5, 1.5, and 2.0.

Keywords: *Graphitic Carbon; Biocompatibility; Epoxy; Mechanical Characteristics; Composite; Photography.*

1.0 Introduction

Graphene's remarkable mechanical and thermal qualities have led to its widespread application as a rein- forcements in polymer composites since 2004 [1]. Graphite has gradually shown itself as a viable replacement for carbon nanotubes (CNT) as a filler in polymers for the overall enhancement of material, electrical, and thermal characteristics of nanomaterials [2, 3]. Gra- phene consists of a 2-D hexagon network containing sp2 hybridized carbon atoms. Graphene's (experimentally calculated and expected) remarkable characteristics and anisotropic [4, 5] behavior are best summarized as follows:

- Percentage elongation and fracturing strength were measured at around 32 and 120 MPa, respectively, for produced graphene (GO) by Dikin et al. [6].
- Employing atomic force microscopy, Lee et al. [7] determined graphene to have the highest tensile strength of any material tested, at 130 GPa (AFM). Additionally, they revealed that the rigidity of single-layer exfoliated graphene was over 200 times that of steel and the stiffness was 1 TPa.
- Mono exfoliated graphene has a rigidity of roughly 0.5 TPa, as analytically measured by Frank et al. [8].

In addition to actual studies of graphene's characteristics, several molecular dynamics simulations of graphene's mechanical characteristics have been undertaken. Tsai and Tu [9] used MD modelling to determine the Young's modulus of graphite and graphite flakes, finding values of 0.912

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and 0.795, respectively. To create a composite material, Sharma et al. [10] used MD to combine graphene, carbon nanotubes, and a metal matrix. They foresaw that Young's modulus would decrease as temperature rose. Both the Young's modulus and the heat capacity of materials containing nanofiller have been investigated. There have been very few reports of experiments using two-phase amine functionalized graphene nanocomposites. This was because of issues in measuring and evaluating graphene and epoxy, due to their anisotropic and non-homogeneous properties.

Table 1: Concordance between the Predicted and Experimental Values of Young's Modulus

Refs.	Category of Graphene	Method	E (TPa)
[7]	Graphene	Experimental	1.2
[12]	Graphene	Experimental	1.2
[12]	Graphene	Ab initio	1.08
[13]	Graphene	Ab initio	4.02
[14]	Graphene	Ab initio	1.2
[15]	Graphene Nano papers	Ab initio	1.66
[16]	Graphene Nanoribbons	MD	1.4±0.05
[17]	Graphene	MD	0.97-1.2
[18]	Graphene	MM	3.8
[19]	Amine functionalized gra-phene	MD	0.78
[19]	Graphene Oxide	MD	0.55
[9]	Graphene and graphite flakes	Experimental& MD	0.717 & 0.915

This highlights the need of learning about the production and characterization of two-phase composites including functionalized graphene, as well as how these factors affect mechanical performance. Using probing and ultrasonication techniques, the authors of this work created an epoxy nanocomposite that was reinforced with amine-functionalized multilayer graphene layers (AF-MGL). Initial steps included creating samples with volume fractions from 0 to 2.0 wt. percent. Tensile strength and flexural strength testing will be done in the next phase. To complement the research investigation, Simulation results were developed to mimic the thermodynamic and elastic characteristics of AF-MGL/EpC. These simulations ran alongside the actual experimental study. Furthermore, the experimental results obtained were compared to the simulation findings.

2.0 Types of Research Methods

2.1 Materials

To create these composites, a percentage of AF-MGLs (from 0% to 2.0% by weight) was mixed to LY556 epoxy resin (phase1) (phase 2). United Nanotech Innovations Pvt. Ltd. of Bangalore, India supplied commercially accessible amine functionalized graphene. Table 3 provides a summary of the many observable qualities of the acquired AF- MGLs.

From Chemanol Industries Ltd. in Mumbai, India, we were able to get the epoxy resin LY556 and the aromatic anhydride hardener HY5200. Density of the neat resin was 1.12 to 1.23 g/cc, and its transition temperature (Tg) was 124 to 146 degrees Celsius.

Doi: 10.51976/jfsa.221909

2.2 Processing for nanostructure

Ultra - sonic Baths Prototype RK100 H, Bandelin, Germany, was used to mechanically mix LY556 epoxy resin with AF-MGL (0.5, 1.5, and 2.0 wt percent) in a beaker for 8-9 minutes. The resulting concoction was sonicated in a probe Ultrasonicated type VCX500 for 1 hour and 15 minutes at 40% amplitude and 30s on/ 20s off cycle pulse mode. The used ultra sonic liquid processor features a 12 mm tip diameter, 500 watts maximum power output, and a 20 kHz working frequency. Furthermore the combination of AF-MGL and epoxy were ball milling at 160 rpm for 2h 40min for homogeneous distribution of nanocomposites. The hardener HY951 was also added with ball milled mixture, and then the combination was further ball milled for 40 min at 160 rpm. Afterward, the mixture was degassed in a vacuum oven for 1 hour and 30 minutes at 70 degrees Celsius. Chamber capacity (L/cu ft) 28/1.0, nozzle size (mm/inch) vacuum 10/0.4, vent 10/0.4, and operating temperature (T) (+5) above room temperature to 250°C describe the OV 11 vacuum oven.

Finally, the AF-MGL/Ep combination was cured at 115°C for 1 hour and 40 minutes, followed by a post cure at 195°C for 2 hours and 40 minutes, all while under vacuum. The mixture is placed into an acrylic mould to prepare the samples for description according to the criteria given by ASTM. One sample of plain epoxy was made, and other samples containing AF-MGL/EpC dispersion at 0.5, 1.5, and 2.0 weight percent were also created for this investigation. Different codes to indicate the wt percent of AF-MGL/EpC are presented in Table 4. A full procedure utilized for fabrication has been depicted in Fig. (1). (1). Last but not least, five samples of each AF-MGL/EpC nanocomposites were cut to the specifications established by the ASTM D3039 and DMA2980 for stress and thermo-mechanical testing, respectively. Table 3 details the dimensions and specifications for the moulds required to produce an item that conforms to ASTM standards.

Table 2: Observational and Anticipated Young's Modulus of Graphene-reinforced Polymer Nano-composites

Refs.	Type of Nanocomposites	Method	E (TPa) (% □)	Tg (^{0}C) (% □)
[34]	graphene/epoxy	Solution	37	-----
[35]	graphene/poly vinyl chloride	Sonication	58	3.5
[36]	graphene/epoxy	Solution	17.3	7.4
[37]	graphene nano-sheets/polystyrene	In-situ	-----	8
[38]	graphene oxide (GO)/polyurethane	In-situ	48.6	3.3
[39]	graphene oxide (GO)/polyimide	In-situ	27	-----
[40]	graphene/CNT/polyethylene	MD	50.5	46.8
[41]	graphene oxide paper/polymer	MD	76.5	-----

2.3 Dynamic mechanical system

By maintaining the specimens at elevated temperatures while subjected to a pure cyclic loading, the glass transition temperature (Tg) of AF-MGL/EpC nanocomposites can be determined by a dynamic mechanical system. Data on the amount of energy retained by nano-composites following deformation was thus obtained. The DMTA samples measured 1.5 by 10.8 by 30 mm3.

Figure 1: Schematic Representation of the Creation of AF- MGL/EpC Nanocomposites

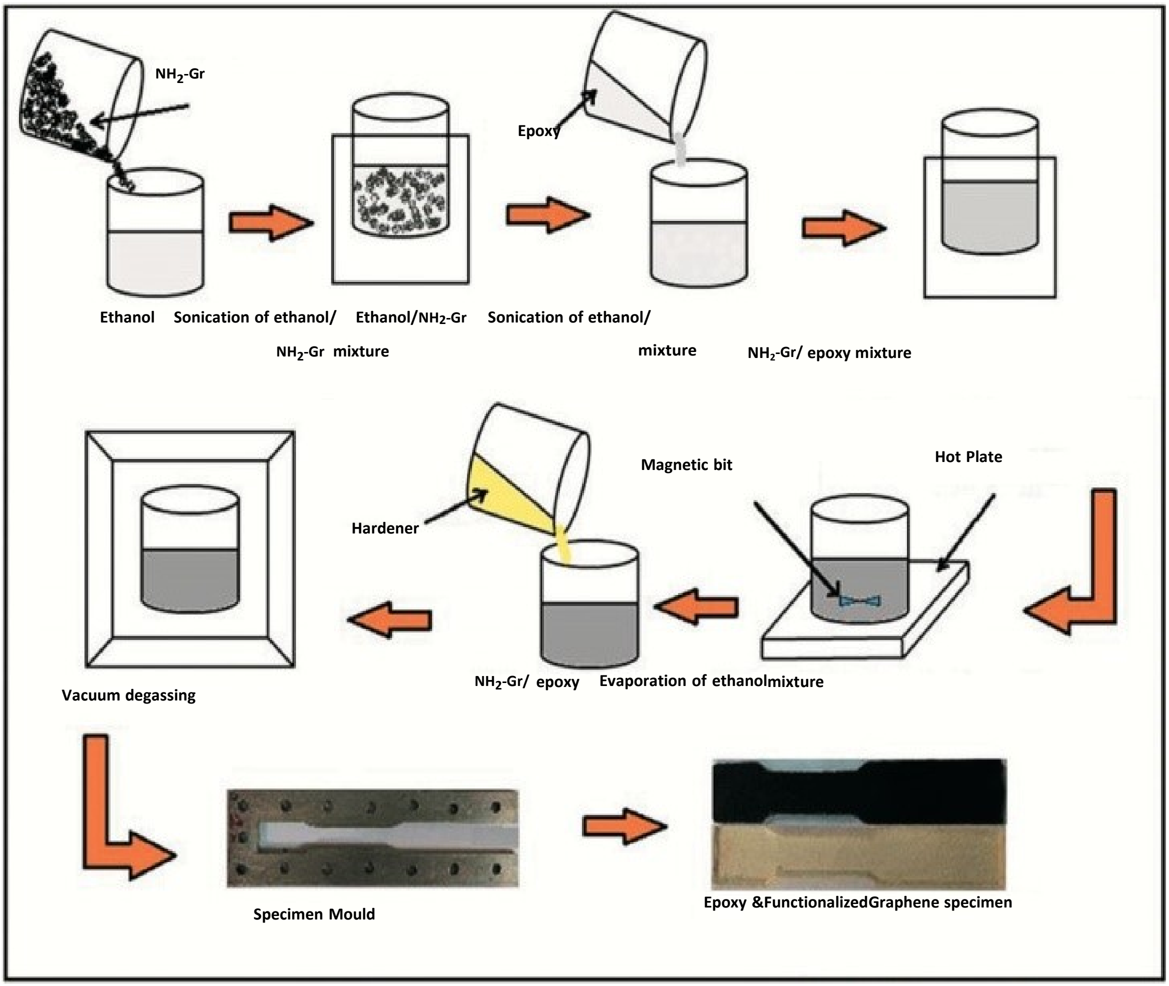


Table 3 Specifications for the Moulds Utilised in This Study

Sr. No.	Specifications	Dimensions (mm)
01	Overall Length	185
02	Gage Length	50
03	Gage width	14
04	Thickness	5
05	Width of grip section	19

3.0 Molecular Simulation and Dynamical Designs

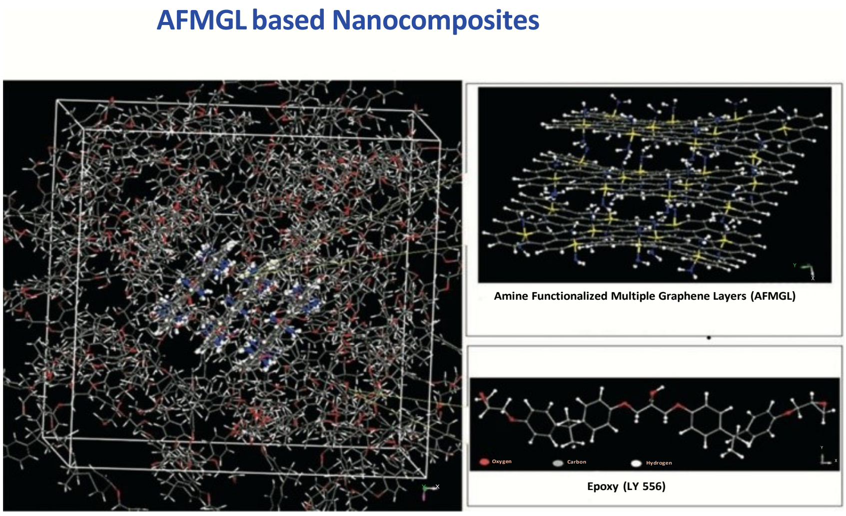
Similar to quantum chemistry, the technique of molecular dynamics was employed to examine molecules at the atomic level. Progressive boundary conditions allow the unit cell to take on the characteristics of the bulk environment, leading to more precise molecular models. It is advised to construct a supercell with specific proportions in the Z-direction to achieve the desired aspect ratio of the 2D graphene sheet (an aggregate of up to 10 microns). If the required aspect ratio is lacking, this strategy may be used. The results of the Simulations were also heavily influenced by the force field choice.

Doi: 10.51976/jfsa.221909

3.1 AF-MGL molecular structure

Structures of several MD constituents are presented in Fig (2). Multiple graphene layers (MGLs) with desirable mechanical properties were finding widespread usage in composites. Model and representation of the MGL block with three carbon sheets (70.56473.342) stacked in a 1-2-1 pattern (Fig (3). For the reinforcing filler in the composites, scientists settled on a single sheet of graphene, which has 228 carbon atoms in all. The inter-planar distance between the carbon fibre sheets was 3.5 [39], and the sheets were positioned such that they overlapped in the centre of the simulation cell (see Fig (3). Since it was assumed that the AF-MGLs were uniformly distributed in the epoxy matrix, the graphene surface was functionalized with a di-ethyl amine group (-NH2).

Figure 2: Stacked Order of the AF-MGL used as filler in AF-MGL/EpC Nanocomposites for Reinforcement



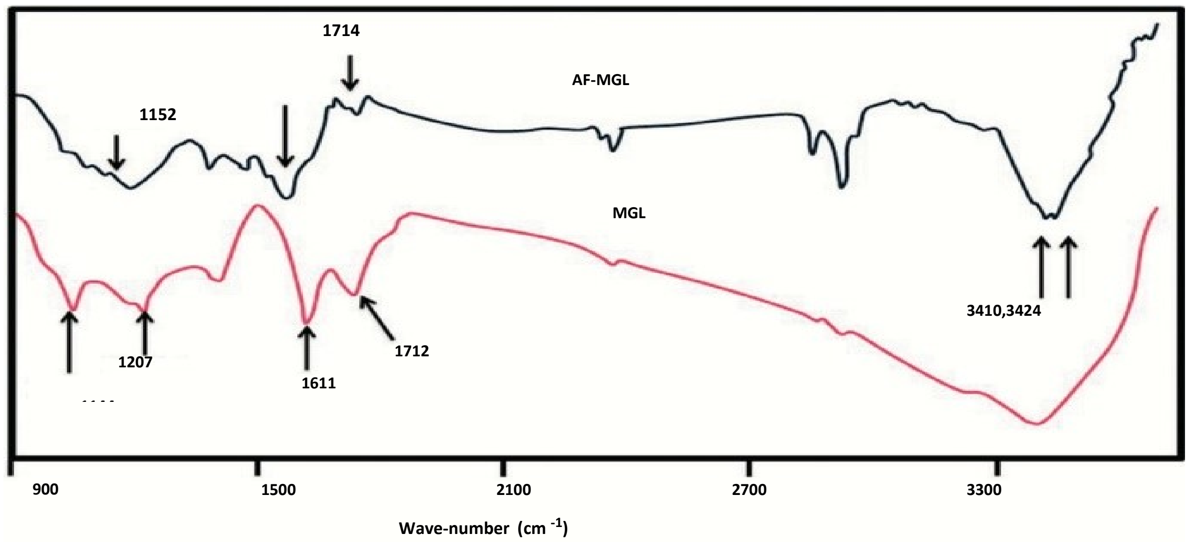
3.2 Epoxy two-phase composite (AF-MGL)

The mechanical properties of cured epoxy resin and a segment of stereochemistry (6, 6) AF-MGL were modelled using MD simulations to identify the two-phase AF-MGLs/EpC nanocomposites. Models of two-phase nanocomposites generated using the equilibration method are shown in Fig (3). Presented in this diagram is a two-phase nanocomposite housed in a supercell with measurements of 78 x 78 x 78. Epoxy resin, with an original density of 1.2 g/cc, was distributed arbitrarily all across surface of AF-MGL to initiate the configuration. The first arrangement resulted from this process. All four possible AF-MGL weight fractions (0.0, 0.5, 1.5, and 2.0) were considered. The term "weight ratio" refers to the amount of AF-MGL to epoxy resin.

4.0 Results and Discussion

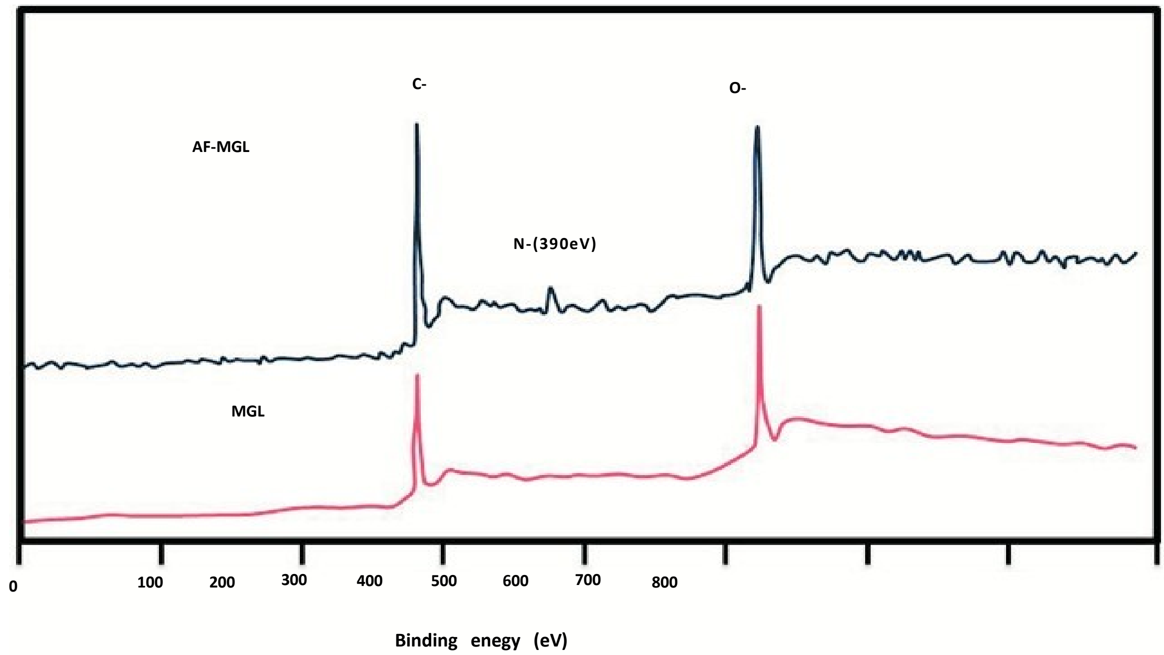
Before anything else, FTIR spectroscopy was used to look for evidence of amine functionalization in MGLs, and it was found. Six samples of both types of AF-MGL/EpC nanomaterials were tested for tensile and viscoelastic properties in the study's second half. Next, we ran simulations on several AF-MGL/EpC nanocomposites to get a sense of their tensile and viscoelastic properties. The last process included analyzing and comparing the experimental and simulated data.

Figure 3 (a) FT-IR Spectra of Unmodified and Amine-functionalized Graphene



The NH2 stretch is shown by the 3424 cm-1 peak in Figure (3a), while the NH2 in-plane stretch is indicated by the 1634 cm-1 peak and the C-N bond stretch is illustrated by the 1188 cm-1 peak. XPS analysis was used to delve into the chemical composition of AF-MGLs. The AF-MGL and MGL survey spectra are shown in Fig (3b). Similar to MGL, carbon and oxygen are present in the survey spectra of AF-MGL, however unlike MGL, nitrogen is also present (3b).

Figure 3 (b) Analyzing the Chemical Composition of AF-MGL using XPS



When a little quantity of AF- MGL was added to the epoxy matrix, it helped to boost the material's mechanical qualities as a whole. In order to do this, we analysed five samples of each specimen code (given in Table 3) to determine the results. In Fig. 4 we see representative stress-strain

Doi: 10.51976/jfsa.221909

curves for MGL and the associated composites. 1.5AF-MGL/EpC (six samples A,B,C,D, and E) was found to provide the best results of all nanocomposites created for this study, hence its findings are shown in Fig. (4). Average scores of tensile modulus and strength for the tested specimens are shown in Figs. (5a) and (5b), together with standard deviation error bars.

Figure 4: Stress-strain Diagram Typical of 1.5 Weight Percent 2AF-MGL/EpC

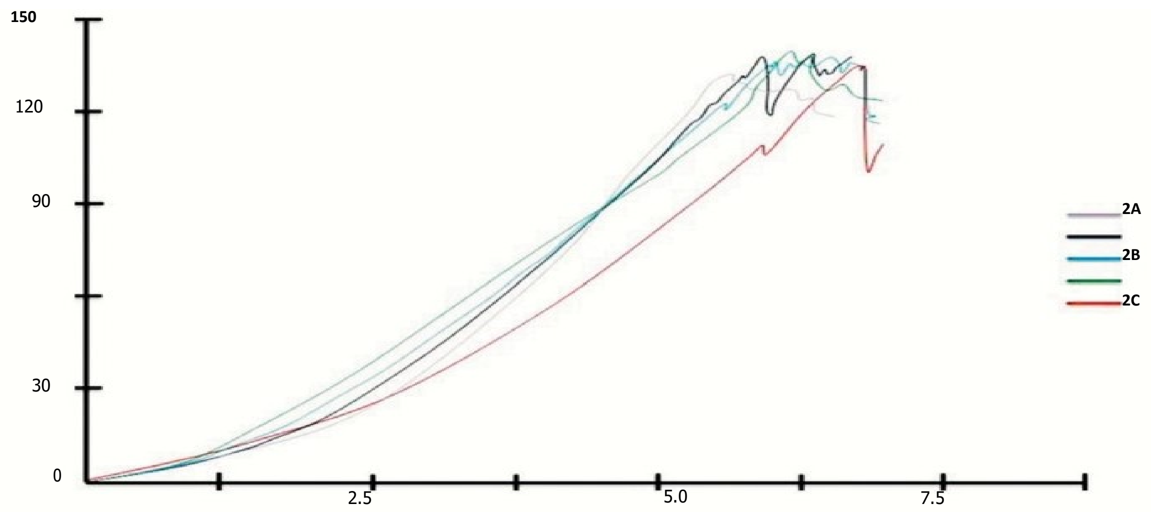
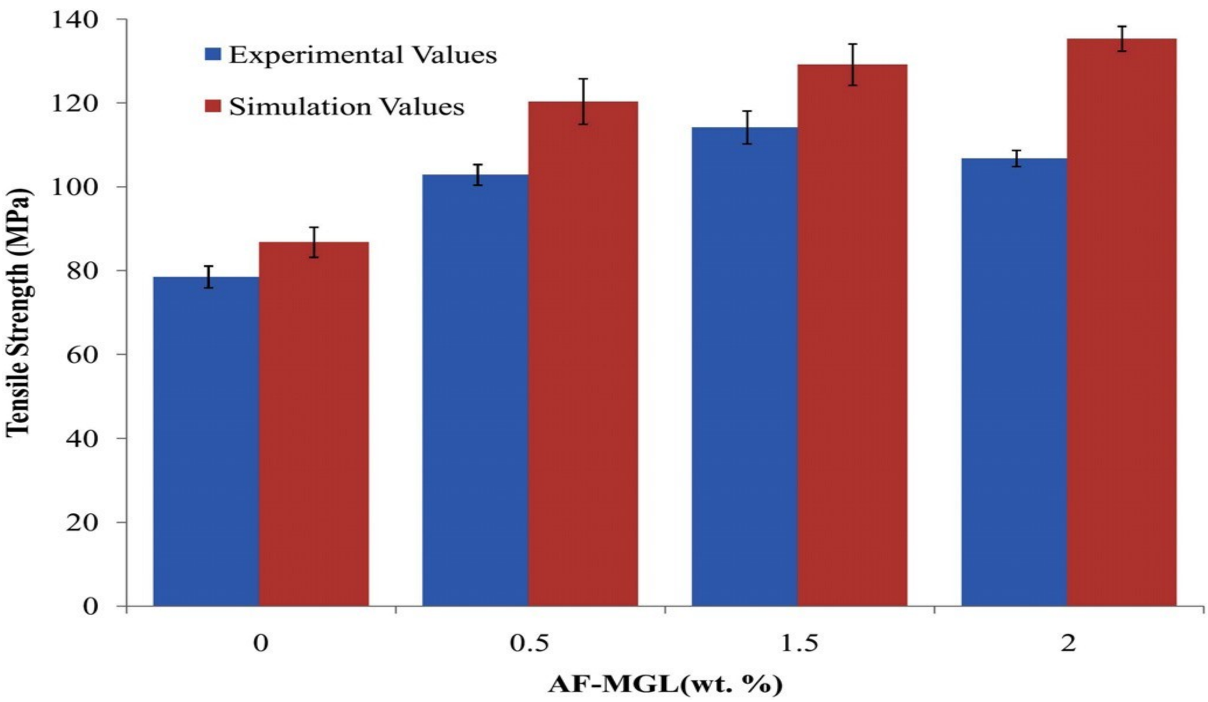
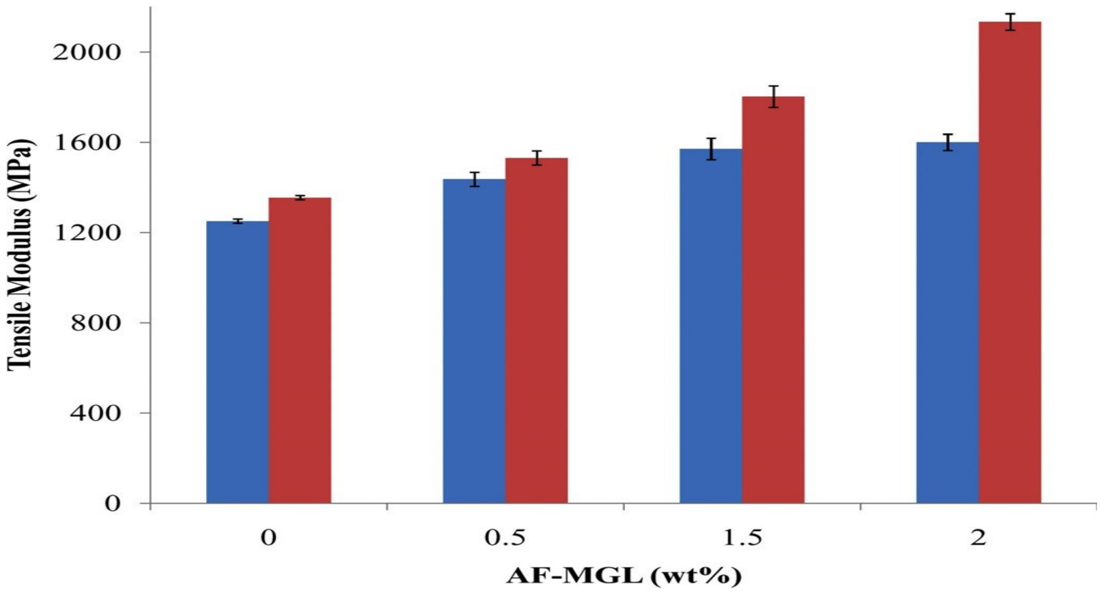


Figure (4): As a Function of the AF-MGL Weight Fraction in AF-MGL/EpC, the Results for (a) Tensile Strength and (b) Tensile Modulus are Shown Below

(a)



(b)



5.0 Conclusion

Improved tensile modulus, strength, and glass transition temperature were among the properties of AF-MGL/EpC nanocomposites that were studied for this article. In this study, AFMGLs were blended into an epoxy matrix at concentrations ranging from 0 to 6.0 weight percent. This study used a holistic method to compare simulation and experimental data for the aforementioned features of two-phase com- posites. The longitudinal tensile modulus and tensile strength of AF-MGL/EpC nanocomposites were enhanced when the epoxy resins were modified with AF-MGL. All of the mechanical characteristics of the AFMGL/EC epoxy nanocomposites were also evaluated using MD simulations. Micrographs taken using a scanning electron microscope (SEM) reveal that the interfacial contact between AF-MGL and the epoxy matrix is significantly enhanced in mechanically tested AF-MGL loaded samples compared to EpC.

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