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Comparative Analysis of Mechanical Response in Epoxy Nanocomposites Reinforced with MXene and Other Carbon-Based Nano-Fillers: An Experimental and Numerical Study

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ABSTRACT

This research introduces a finite element model tailored explicitly to assess the mechanical characteristics inherent in MXene/polymer nanocomposite. The primary focus revolves around elucidating the performance attributes through numerical simulations and subsequently aligning these findings with experimental data. The numerical analysis not only predicts mechanical behaviours but also aims to correlate these insights with experimental results obtained from fabricated epoxy nanocomposites within the study's scope. By employing this simulation-driven approach, the study investigates a deeper understanding of the mechanical response, particularly focusing on the materials' tensile properties. From the experimental results, the MXene/epoxy nanocomposite sample exhibited the highest tensile strength and modulus, measuring 50.1 MPa and 7.13 GPa, respectively. The simulation results were 50.08 MPa and 6.95 GPa, showing a difference of less than 3%. Small discrepancies in Young's modulus between the experimental and simulation results may arise from inherent sample heterogeneity. This heterogeneity, which includes microstructural variations, impurities, or defects, contrasts with the idealized homogeneous structures assumed in simulations. This research endeavours to advance predictive modelling techniques, offering valuable insights that can potentially streamline the manufacturing process and optimize MXene-based polymer composites. The goal is to tailor these materials with precise mechanical properties, ensuring their enhanced performance in various applications.

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1. Introduction

Recently, polymers have gained significant attention [1] due to their ease of production [2], lightweight nature, flexibility, and cost-effectiveness [3]. Incorporating nanomaterial fillers expands the range of customizable traits, resulting in new composite materials with various functions suitable for uses in energy storage [4], shielding against electromagnetic interference [5], coating [6] and aerospace [7].

MXenes, a broad category of two-dimensional (2D) materials introduced in 2011, have drawn considerable interest for their unique properties [8]. These include high metallic conductivity, impressive mechanical characteristics, and hydrophilicity arising from surface modifications post-etching [9]. These qualities position MXenes as strong candidates for crafting innovative polymer composites with diverse functionalities including energy storage [10]. The research and development in MXene-based energy storage devices continue to expand, showing promise for addressing the growing demands for efficient and sustainable energy storage solutions [11,12].

Over 40 variations of MXenes have emerged, potentially surpassing the popularity of other 2D materials such as graphene [13]. Initially, hydrofluoric acid was used to selectively remove layers of transition metal carbides and carbonitrides from the MAX phases, marking the beginning of MXenes. Subsequently, various synthesis methods have been developed, including selective etching in fluoride salt solutions, non-aqueous etchants, halogens, and molten salts [14]. These techniques have enabled the creation of new MXenes, enhancing control over surface chemistry.

Researchers have focused on enhancing the properties of epoxy nanocomposites while maintaining their structural integrity [15]. Unlike traditional filled epoxy composites, achieving this improvement requires only a small amount of dispersant, resulting in significant enhancements across various traits like tensile strength, glass transition temperature, impact resistance, interlaminar shear strength, and flexural test values [16]. Numerous studies have reported improvements in the tensile properties of polymers incorporated with MXenes. Che Nasir *et al.*, found that MXene/epoxy nanocomposites resulted in a significant enhancement of tensile strength and elastic modulus, with increases of up to 66.57% and 22.65%, respectively, compared to neat epoxy [16]. Saharudin *et al.*, suggest that MXene materials could significantly improve tensile strength and modulus by 314% and 89%, respectively, when incorporated into a polymer matrix [7]. In another study conducted by Gong *et al.*, Young's modulus and tensile strength of epoxy were increased by 743% and 91%, respectively [17]. This improvement can be attributed to the effective stress transfer between the matrix system and the MXene sheets, resulting in enhanced mechanical properties.

Additionally, nanocomposite coatings provide a practical solution for enhancing corrosion resistance, as highlighted by recent research [18]. Polymer nanocomposite coatings, renowned for their outstanding qualities, have sparked considerable interest in corrosion prevention. Within polymeric coatings, epoxy resin stands out prominently because of its exceptional chemical and corrosion resistance [19], dimensional stability, adhesion, high tensile strength, and minimal shrinkage post-curing [20].

This research project aims to develop numerical simulations using the ANSYS2023 commercial finite element package to study the mechanical behaviour of an MXene epoxy nanocomposite. Notably, discussions regarding the numerical simulation of MXene/epoxy composites are limited in existing literature. This research endeavour aims to fill this gap, providing new insights and advancing knowledge specifically for energy storage applications. Comparing mechanical responses in MXene-reinforced epoxy nanocomposites with other carbon-based nano-fillers offers essential insights for choosing nano-fillers to improve material properties. The integration of experimental data and

numerical simulations informs the development of advanced nanocomposites with specific mechanical characteristics.

2. Methodology

2.1 Materials

A liquid epoxy (EL2) and hardener were purchased from Easy Composite in Stoke-on-Trent, UK. The liquid epoxy exhibits a viscosity range of 12.0-15.0 cP, while the hardener registers a viscosity between 10.0-12.0 cP at 25°C. The epoxy mixture was prepared by combining the epoxy and hardener in a weight ratio of 2:1.

In this study, four distinct nanofillers were employed: MXene, Graphene nanoplatelets (GNPs), and carbon nanotubes (CNTs). The GNPs, having a particle size of 2 µm and a thickness ranging from 0.4 to 1.7 nm, exhibit a specific surface area of 300 m²/g and 99.2% purity. The CNTs measured 0.5-10 µm in length and 7-15 nm in diameter. Both GNPs and CNTs were purchased from Sigma-Aldrich, UK, while the MXene, modified to have a thickness between 1.2 and 1.8 nm, was acquired from Nanoshell, India.

2.2 Fabrication of Nanocomposite Samples

Nanofiller samples weighing 0.1 wt.% were measured using an analytical balance and gently mixed with the hardener manually for 30 seconds. Subsequently, they underwent 30 minutes of sonication at room temperature using a water bath sonicator. After cooling the suspension back to room temperature, it was combined with liquid epoxy at a 2:1 ratio of epoxy to hardener. Thorough hand mixing continued for an additional 5 minutes before pouring the mixtures into the mould (Figure 1). These samples were then left to cure at room temperature for 24 hours before undergoing a post-curing process at 90°C for 5 hours to ensure complete cross-linking. A mixture ratio of 40 parts silicone rubber to 1 part curing agent was poured into the acrylic moulds and left for 24 hours to complete the curing process. The tensile test specimens adhered to the ASTM D638 Type V standard (Figure 2), and the testing procedure was conducted at a crosshead speed of 1 mm/min.

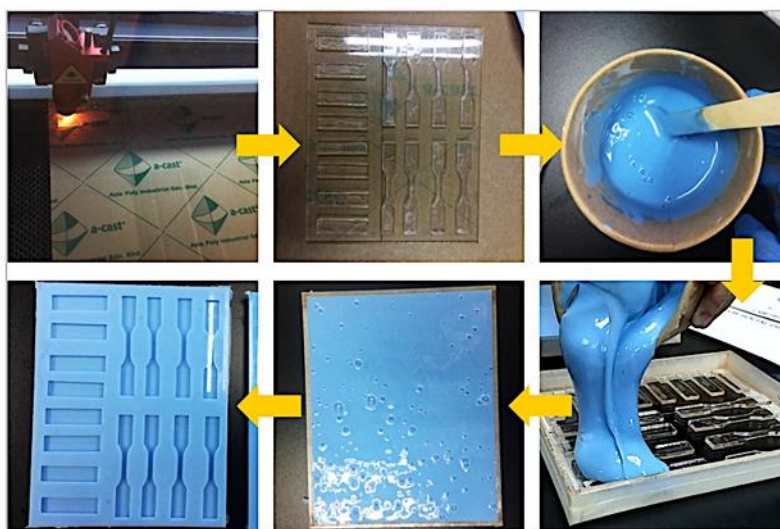


Fig. 1. Silicone mould preparation

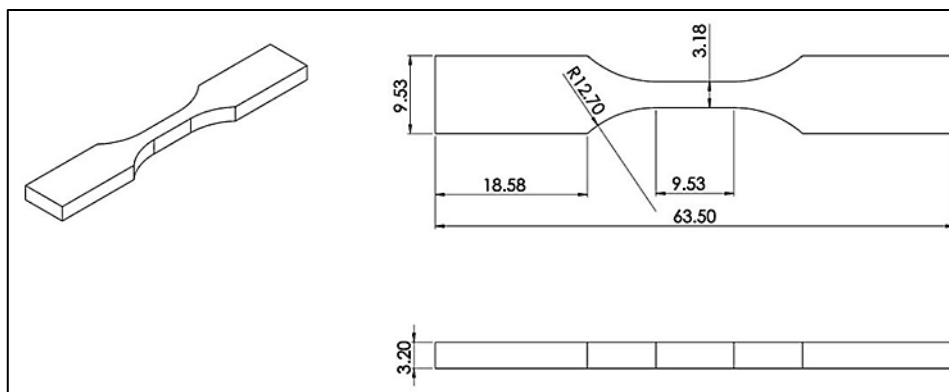


Fig. 2. Tensile test dimensions according to ASTM D638 (type V)

2.3 Bilinear Isotropic Hardening Properties of Neat Epoxy and Nanocomposite Samples

The Bilinear isotropic hardening properties that were used in the simulations are shown below in Table 1. Bilinear isotropic hardening pertains to how a material behaves when subjected to plastic deformation, specifically in the realms of tensile properties. The term "bilinear" indicates that the connection between stress and strain is characterized by two separate linear segments.

Table 1

Bilinear isotropic hardening properties

Material	Young's modulus, E (Pa)	Tangent modulus, E_t (Pa)	Density (nanomaterial)	Poisson's ratio, ν
Epoxy	5.86E+9	4.06E+9	1.16 g/cm ³	0.35 [16]
CNTs	6.34E+9	1.16E+9	1.3 g/cm ³	
GNPs	6.52E+9	1.95E+9	2.1 g/cm ³	
MXene	7.13E+9	1.97E+9	4.21 g/cm ³	

2.4 Scanning Electron Microscopy

In this study, SEM (Scanning Electron Microscopy) was utilized to examine and analyse the dispersion of the nano-filler within the matrix, as well as to investigate the interface and any potential interphase attraction between these components. Additionally, the fracture surfaces of the samples subjected to tensile loading were observed using SEM. Sample sections were cut and secured onto stubs using copper tape, then coated with silver using a Quorum Q150T ES machine.

2.5 Numerical Analysis

ANSYS2023 stands out as an effective resource for conducting design analysis. Among various solutions for intricate analyses, the finite element system stands as a comprehensive approach. Analytical solutions often fall short in addressing engineering complexities arising from intricate material properties, diverse boundary conditions, and the structure's inherent intricacies. Hence, the finite element method relies on assembling subdivisions, termed finite elements to represent bodies or structures. This method effectively transforms problems based on partial differential equations into a system of linear algebraic equations, as depicted in Eq. (1).

$$[K]\{q\} = \{F\} \quad (1)$$

where K is the stiffness matrix, q is the Nodal displacement vector and F is the Nodal vector force Utilizing ANSYS2023 involves a procedural approach encompassing Geometry and Element types. To conduct analyses, material properties such as Young's modulus, Poisson's ratio, density, alongside boundary and load conditions, mirror those of the experimental setup [21]. In structural scenarios where thickness is significantly smaller compared to length and width, shell elements find common applications.

In ANSYS2023 Workbench software, static structural analysis simulations were conducted with one end fixed [22]. The boundary conditions set for these simulations were as follows: a fixed support at the left end and a force range from 420N to 510N, derived from experimental data. Meshing was performed automatically without refinement or specific sizing studies, resulting in 564 nodes and 63 elements.

To account for the non-linear behaviour observed in the curve, the bilinear module was applied atop the linear isotropic condition [23]. In a bilinear module, tangent modulus E_t is shown in Figure 3. This bilinear model approach aimed to accurately capture the material response, considering its non-linear characteristics, during the simulations [24].

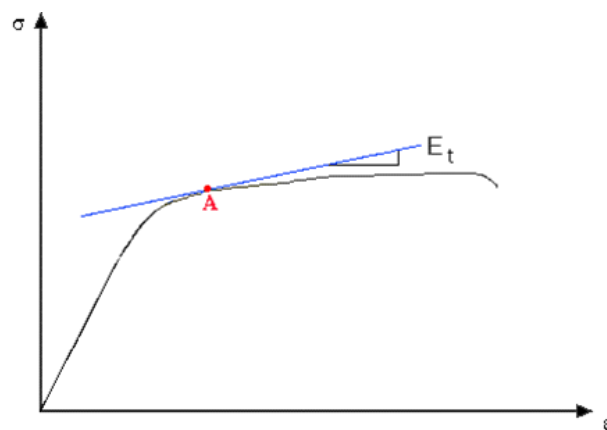


Fig. 3. Tangent modulus E_t at the stress-strain curve

3. Results and Discussion

3.1 Mechanical Characterization: Tensile Testing

The stress-strain curve presented in Figure 4 displays the performance of various nanocomposite samples during the tensile test. Among these samples, the neat epoxy exhibited the least impressive tensile properties. Both the tensile strength and Young's modulus of the neat epoxy were notably lower in comparison to the epoxy/CNTs, epoxy/GNPs, and epoxy MXene nanocomposite samples. This indicates that the addition of CNTs, GNPs, or MXene to the epoxy matrix significantly improved the material's tensile strength and stiffness (Young's modulus) in contrast to the neat epoxy. Figure 5 illustrates the break force of different nanocomposite samples. Among these samples, the neat epoxy demonstrated the lowest break force, measuring at 420 N. In contrast, the epoxy/MXene sample exhibited the highest break force, reaching 510 N. This indicates a substantial increase in break force attributed to the presence of MXene, which surpassed the enhancements observed in both CNTs (11%) and GNPs (20%) composite samples.

When considering the strength-to-weight ratio, this increase in break force associated with the epoxy/MXene composite becomes even more significant. The higher break force with MXene suggests that, in addition to the absolute force endured before failure, the material's strength concerning its weight is notably superior compared to the other nanocomposite variations. This

superior strength-to-weight ratio implies that the epoxy/MXene composite offers enhanced strength per unit of weight, making it a promising choice for applications where both strength and lightweight properties are crucial.

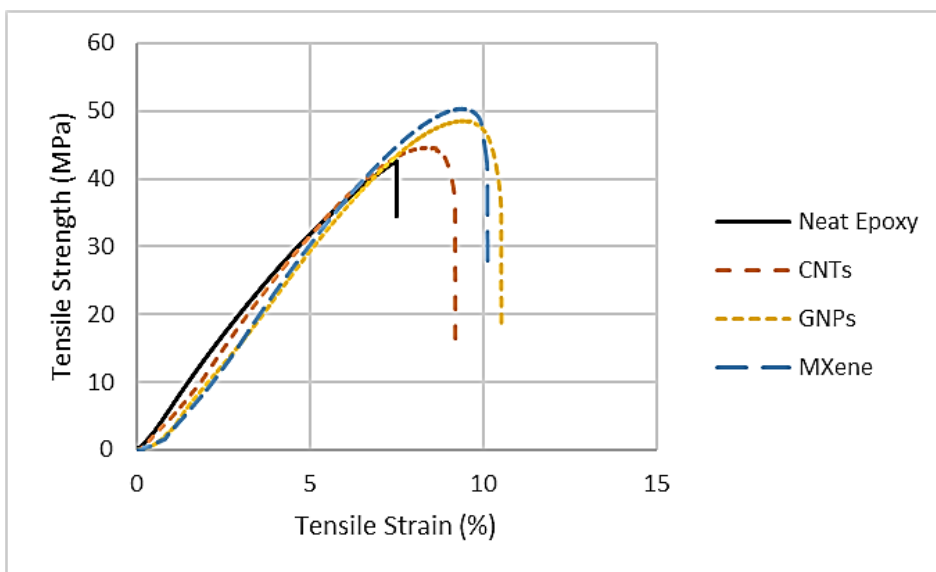


Fig. 4. Stress-strain curves of nanocomposite samples

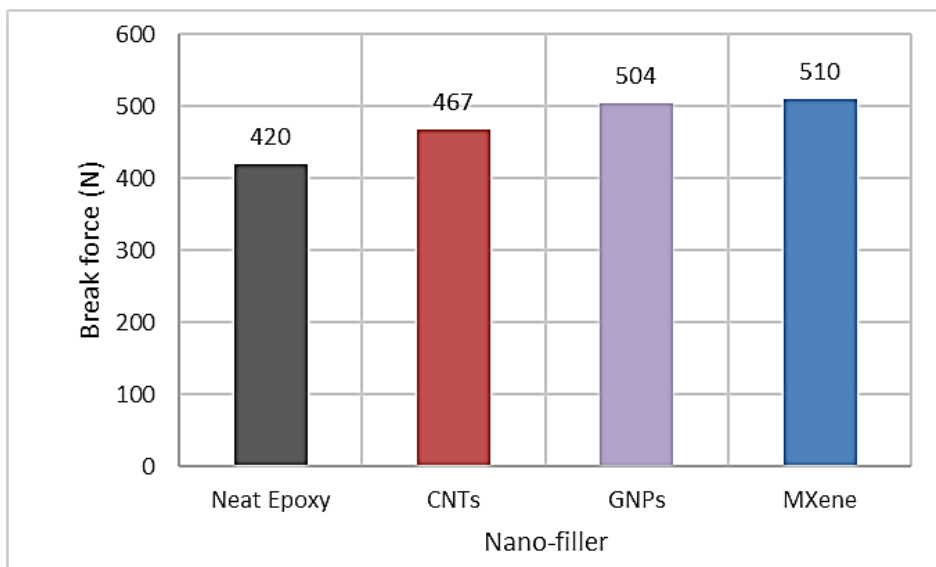


Fig. 5. Maximum force or load applied to a material sample before it fractures

3.2 Numerical Model and Results

The meshing in Figure 6 illustrates the division of the tensile geometry into smaller elements or nodes, enabling a detailed representation of the structure for precise analysis. Meanwhile, the boundary condition depicted in another figure (Figure 7) outlines how the model is constrained or subjected to external forces, crucial for simulating real scenarios and studying the sample's response under specific mechanical conditions.

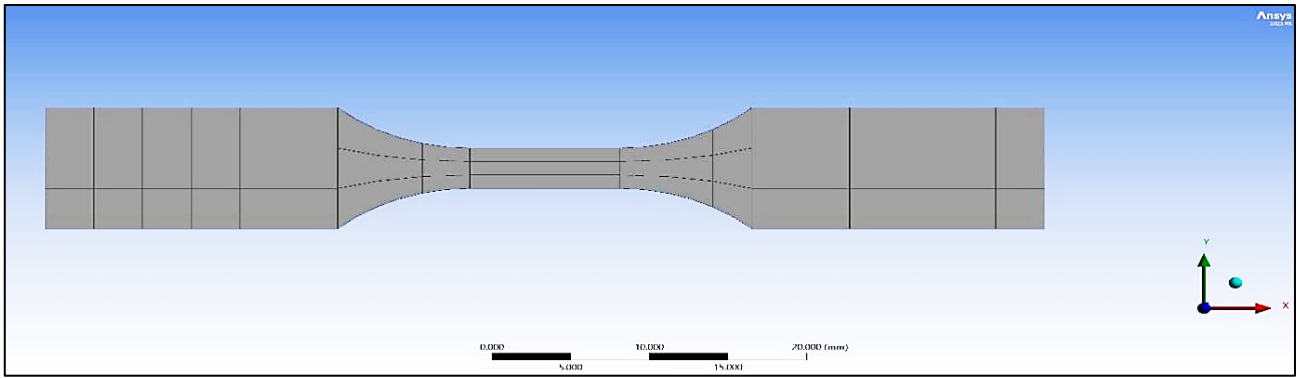


Fig. 6. Mesh of the tensile geometry

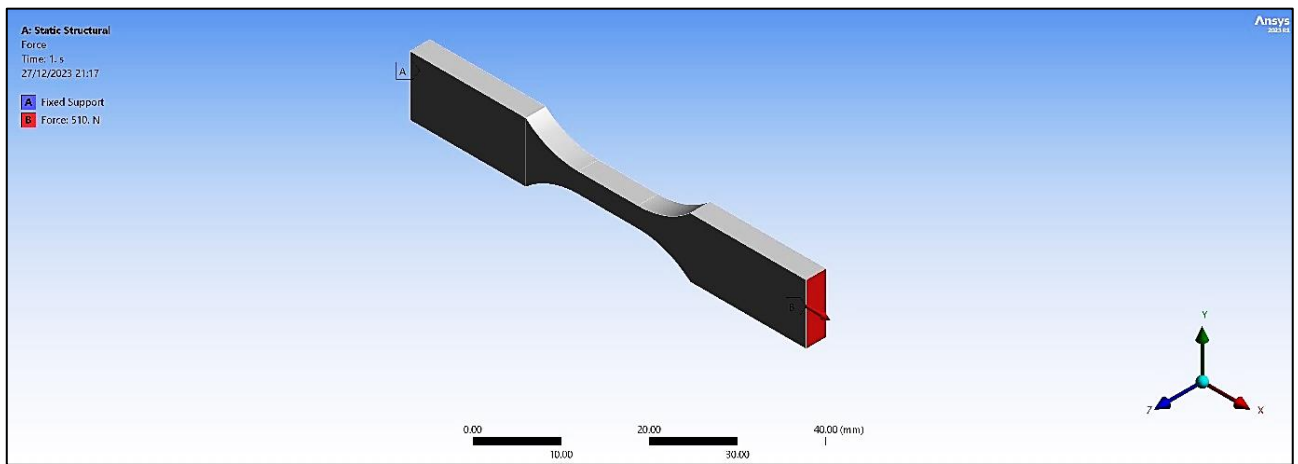


Fig. 7. Boundary conditions

An isotropic and bilinear finite element model was developed to predict the tensile properties of MXene/epoxy nanocomposite and other samples. The maximum stress of all samples is shown in Figures 8 to 11 below.

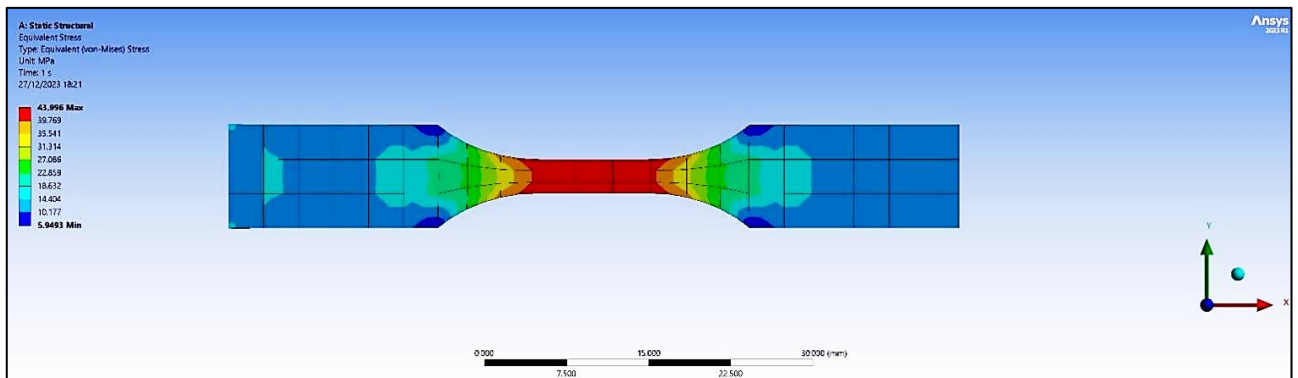


Fig. 8. Maximum stress of neat epoxy sample

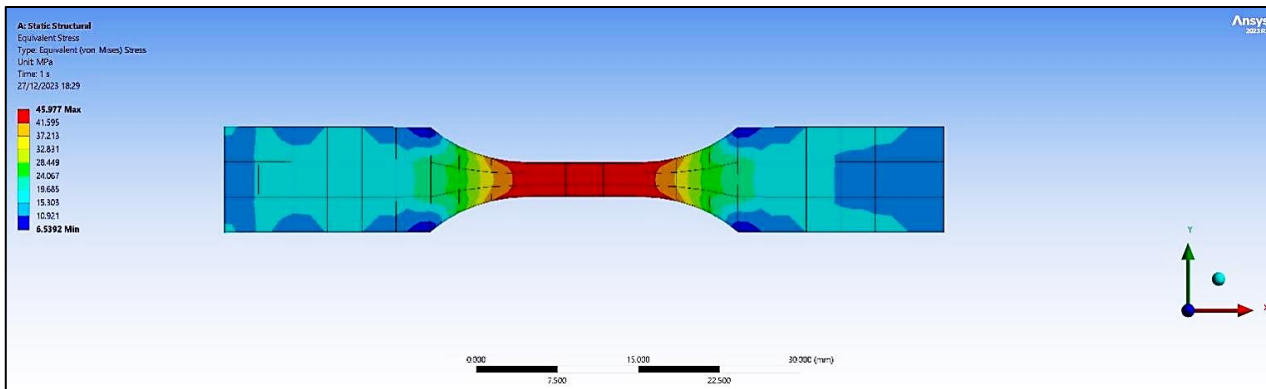


Fig. 9. Maximum stress of CNTs/epoxy nanocomposite sample

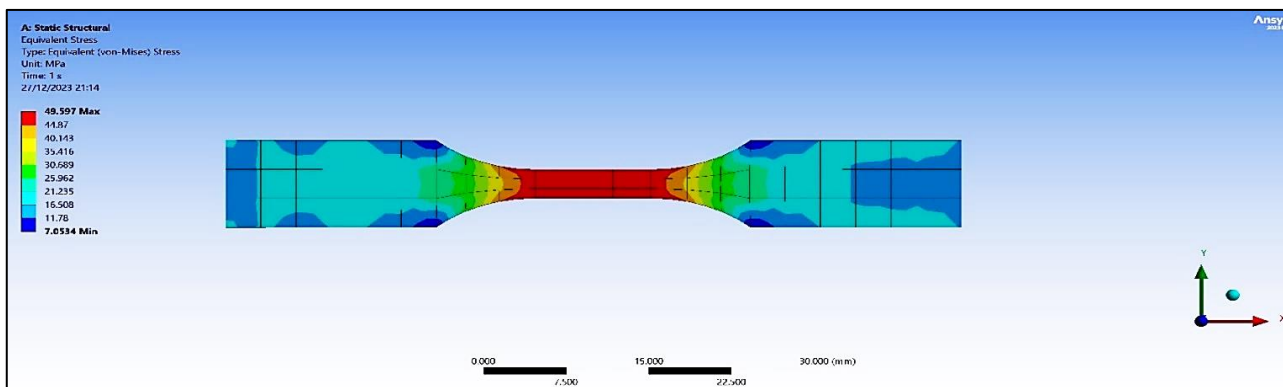


Fig. 10. Maximum stress of GNPs/epoxy nanocomposite sample

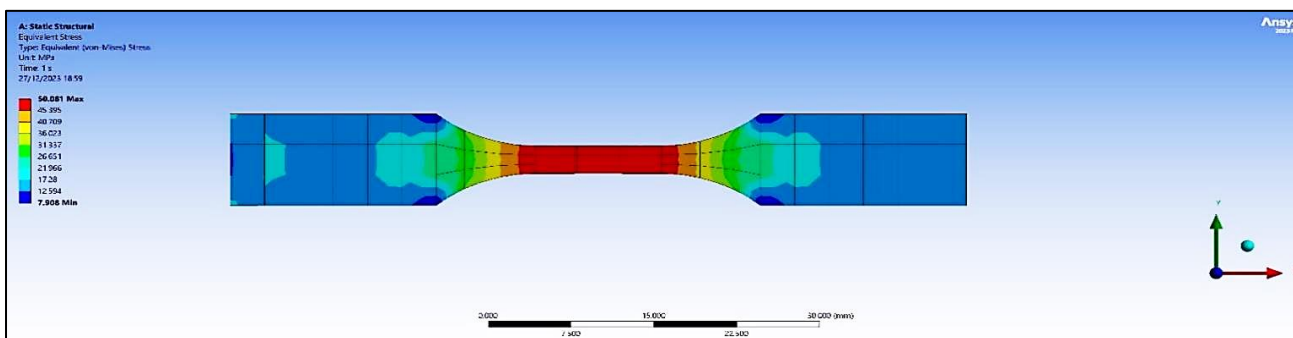


Fig. 11. Maximum stress of MXene/epoxy nanocomposite sample

Tables 2 to 4 present the comparison between experimental and simulation data. Overall, the disparities between the results from experiments and simulations fall within acceptable ranges (below 10%), aligning with findings observed in prior research [25]. A small disparity in Young's Modulus between experimental and simulation outcomes may arise from the inherent heterogeneity present in samples [26]. This heterogeneity, stemming from variations in microstructure, impurities, or defects [27], contrasts with the idealized homogeneous structures assumed in simulations [28]. The existence of such heterogeneity in experimental samples can contribute to the observed differences in Young's Modulus values when compared to simulated results.

Table 2
 Tensile stress test results

Sample/parameter	Tensile stress σ (MPa)		
	Experiment	Simulation	Difference (%)
Neat epoxy	42.63	43.996	3.2
CNTs/epoxy	44.57	45.98	3.2
GNPs/epoxy	48.9	49.6	1.4
MXene/epoxy	50.1	50.08	0.04

Table 3
 Young's Modulus results

Sample/parameter	Young's modulus, E (GPa)		
	Experiment	Simulation	Difference (%)
Neat epoxy	5.86	5.85	0.11
CNTs/epoxy	6.34	6.96	9.88
GNPs/epoxy	6.52	7.05	8.21
MXene/epoxy	7.13	6.95	2.45

Table 4
 Tensile strain results

Sample/parameter	Tensile strain ϵ (%)		
	Experiment	Simulation	Difference (%)
Neat epoxy	42.63	43.99	3.2
CNTs/epoxy	44.57	45.98	3.2
GNPs/epoxy	48.9	49.6	1.4
MXene/epoxy	50.1	50.08	0.04

3.3 SEM Analysis

The SEM (Scanning Electron Microscope) image provided illustrates the neat epoxy sample (Figure 12), revealing a distinctive pattern typical of brittle fracture. This pattern is characterized by prominent cracks and a remarkably smooth surface and line evident within the image. These visible features collectively suggest that; the pure epoxy material possesses inherent limitations in terms of impact resistance and fracture toughness [29].

The presence of significant cracks in the material's structure, as highlighted in the SEM image (Figure 12(a)), points towards its vulnerability to sudden and severe structural failure under stress. Additionally, the smoothness of the fractured surface (Figure 12(b)) suggests a lack of energy absorption and dissipation, which are typically associated with materials exhibiting higher toughness and resilience against fracture [30]. Overall, these observed characteristics in the neat epoxy indicate its predisposition to brittle behaviour, emphasizing its limited ability to withstand impacts or deformation without fracturing.

The fracture surface morphology of the epoxy/MXene nanocomposite (Figure 13(a)) displays a rugged surface marked by striations resulting from alterations in the direction of crack propagation [17]. This indicates the apparent integration of MXenes within the epoxy matrix, forming interfaces between the two phases [31]. These interfaces signify enhanced energy absorption and improved fracture toughness of the nanocomposite [32]. This is indicative of fracture prevention facilitated by robust bonding between MXenes and the matrix.

In Figure 13, it is evident that MXene agglomerates are found within the epoxy matrix. Despite the presence of agglomerates, which reduce load transfer efficiency and impede crack propagation at the agglomerate-matrix interface, the tensile properties remain superior compared to CNTs and

GNPs. The presence of agglomerates (Figure 13(b)) impacts load distribution and crack progression, leading to a reduction in tensile strength. However, despite this effect, the overall tensile properties remain significantly superior compared to those identified in CNTs and GNPs, consistent with findings from previous research [16].

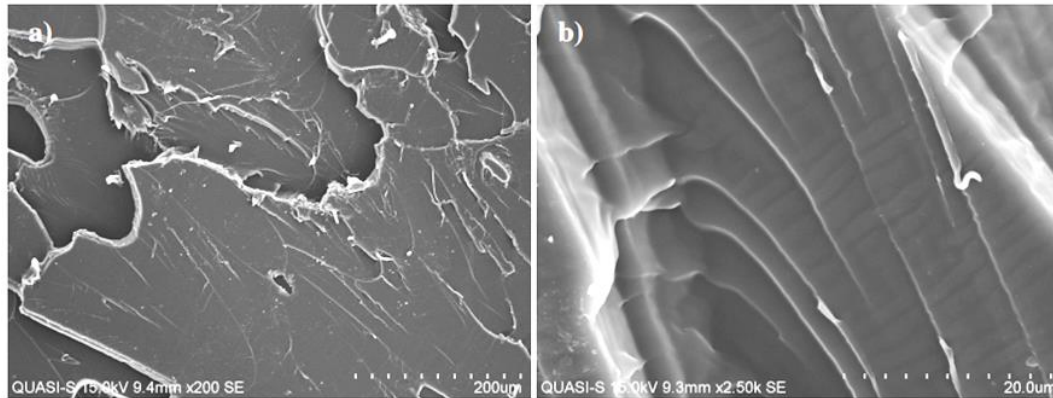


Fig. 12. SEM image of neat epoxy sample

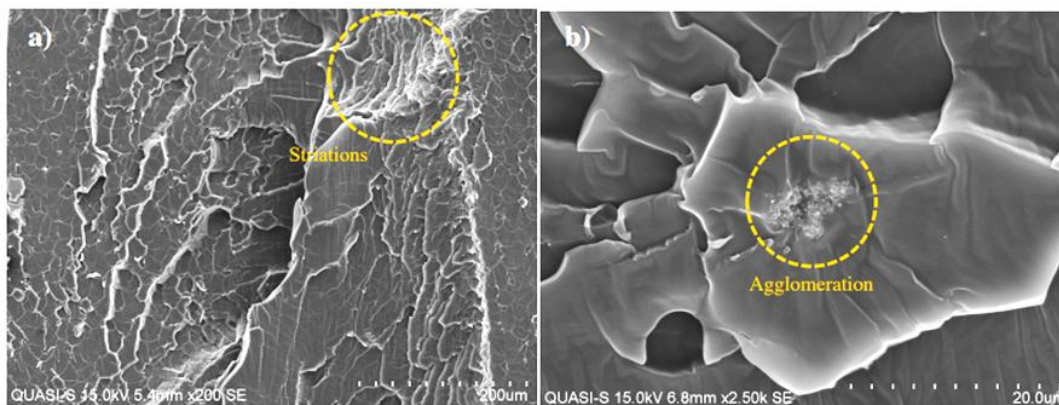


Fig. 13. SEM image of MXene/epoxy nanocomposite sample

4. Conclusion

The research focused on creating and evaluating epoxy nanocomposites utilizing different nanofillers, specifically MXenes, GNPs, and CNTs to understand their impact on reinforcing mechanisms through the matrix of the epoxy composites. The study extensively investigated the tensile properties, including tensile strength, failure strain, and Young's modulus, and compared these experimental results with finite element analysis (FEA) models. The FEA simulations effectively utilized both linear and bilinear models. Notably, the comparison between experimental data and simulations revealed minimal disparities for tensile strength and Young's modulus. However, in the case of tensile strain, the simulation results exhibited discrepancies of up to 24%. Future endeavours may benefit from employing a multilinear model to enhance the accuracy of simulation outcomes. The analysis highlighted that the MXene/epoxy sample exhibited remarkable enhancements, notably presenting a coarser surface. This observation suggests a more robust interfacial interaction between MXenes and the epoxy matrix, indicating potential superior reinforcement capabilities compared to GNPs and CNTs.

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