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# DETERMINATION OF MECHANICAL PROPERTIES OF GRAPHENE REINFORCED TETRA-GEDVA NANOCOMPOSITE

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**Abstract.** In the present study, effects of aspect ratio and perforation on the elastic response of graphene nanosheet (GNS)-embedded Tetra GEDVA (triglycidyl ether of divanillyl alcohol) nanocomposite plate are studied by material studio analysis. A dense amorphous cell is created using the Forcite module and simulation is performed. Young's modulus is predicted at varying strain rates from 0-1 GPa. The study conducted coarse-grained molecular dynamics (MD) simulations of Nano-indentation of PMMA (polymethyl methacrylate) polymer to study the variation of the elastic properties near the interface between the indenter and the substrate. Results have revealed that Young's modulus increases with an increase in reinforcement quantity.

**Keywords:** MD simulation, TetraGEDVA, PMMA, graphene, nanocomposite

## 1. Introduction

The nanocomposite is a strong material where one of the stages has one, a few components of under 100 nanometres (nm). Nanocomposite materials have developed as appropriate choices to overcome the restrictions of micro composites and monolithic while posing preparation challenges related to the control of elemental composition and stoichiometry in the nanocluster phase. These are accounted for to be the materials of the 21$^{st}$ century in the perspective of having plan uniqueness and property mixes that are not found in traditional composites.

Over the previous decade, propelled material specialists had concentrated on the improvement of polymer-based nanocomposites strengthened with well-characterized nanostructured mixes, which are required to give superior materials, with potential application in a wide scope of mechanical regions, for example, defence, aviation, automobile enterprises and so forth. The study was done for current challenges associated with processing and scalability of graphene composites but there is a future perspective for this new class of nanocomposites [1]. Morphology of dispersed graphene and properties from different blending routes are compared TEM (transmission electron microscopy) showed that graphene distributed parallel to the composite surface using the solvent method, while distributed randomly in melt blended method [2]. A specific favourable position of graphene reinforced i.e. high aspect ratio, non-usefulness, better electronic and heat conductivity, thermal stability makes it a potential support possibility for polymer-based nanocomposites. Specifically, epoxy nanocomposites with improved properties (flexible modulus, elasticity, and durability) have acquired by strengthening graphene into epoxy lattice [3], which makes the nanocomposites ideal for medical implants, sports equipment applications [4]. In addition to the improvement in mechanical properties, graphene reinforced nanocomposites often exhibit

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enhanced thermal properties and electrical properties as well [5]. Moreover, graphene-based nanocomposites have unique applications in a broader range of industries. Thin-film capacitors for a computer chip, solid polymer electrolytes for batteries, automotive and aircraft engine parts and fuel tanks, etc. Epoxy resins have the notable class of thermosetting polymers which are broadly utilized as adhesives, electronic encapsulating compounds, covering materials, and the natural period of composite materials because of their high mechanical quality, high concoction consumption and disintegration opposition, phenomenal electrical protection.

TetraGEDVA (triglycidyl ether of divanillyl alcohol) has a bio-based thermosetting epoxy that has new and many of its properties are not known but are like another thermosetting polymer. In this context, various research has been done highlighting the importance of polymer-based nanocomposites and reinforcement of graphene reinforced [6] explored the interfacial mechanical conduct of multi-layered graphene-PMMA layered nanocomposites by performing pull-out recreations utilizing material studio. The outcomes uncovered two unmistakable mechanism failure, pull-out (failure along graphene-PMMA interface) and yielding (failure inside the multi-layered graphene). A one-step cross-linking of epoxy networks was conducted, and it was found that the adopted method was not precise enough to obtain a high percentage of curing compared to that obtained synthetically [7]. The cross-linking mechanism was reported that stated two-stages cross-linking which consists of unstrained and uniaxial strained [8]. The study conducted coarse-grained molecular dynamics (MD) simulations of Nano-indentation of PMMA polymer to study the variation of the elastic properties near the interface between the indenter and the substrate. Characterization of elastic properties was performed [9]. A study was directed on the measure of load move between a graphene sheet and polyethylene on a nanoscale by using the technique for MD reproductions. The creators had presumed that the graphene sheets gave off an impression of being clung to polymer chains in a zone and the interphase layer remained unaffected [10]. The received displaying approaches on epoxy nanocomposites to recognize and penetrate the interfacial conduct and interphase properties. A decrease in interfacial attachment with an expansion in crosslink change was seen between the network and the filler [11]. Li et al. [12] managed multilayer graphene for the examination of the interfacial layer of cross-connected epoxy, concentrating on the different direction of the layers by MD reproductions. The epoxy selected is a new one. It is a synthesized epoxy from vanillin, this bio-based thermosetting polymer also explores the new avenues of composite as its main component (vanillin) is a plant derivative. There has been little work on the mechanical and chemical properties of the compound. The Bio-based epoxy monomers from divanillyl alcohol were successfully synthesized and characterized. It was reported that there is a promising substitute to bisphenol with the aim of designing high-performance epoxy thermosets for structural composite and adhesive applications demonstrating the process and monomers of the cured compound were utilized to make the MD simulations [13]. The addition of graphane with polymer matrix composite has been discussed by the authors. It was proposed that the addition of graphene increase the tensile strength, young modulus, and fracture toughness at the expenses of some decrease in plasticity as compared to pure host polymers [14]. The method of molecular dynamics provides the better results on the nanoscale level as compared to finite elements method during atomistic modeling of the indentation of thin films [15]. In the present examination, molecular dynamics reproduction has been utilized to obtain the mechanical properties of graphene strengthened epoxy nanocomposite. TetraGEDVA has been selected for matrix material. Figure 1 shows the TETRA-GEDVA monomer structure of the selected material. An amorphous cell has been created using a single layer of a graphene sheet by random reinforcement. The Mechanical properties of epoxy nanocomposite have been

determined with and without the reinforcement of the graphene sheet. Figure 2 shows the amorphous model of Tetra GEDVA.

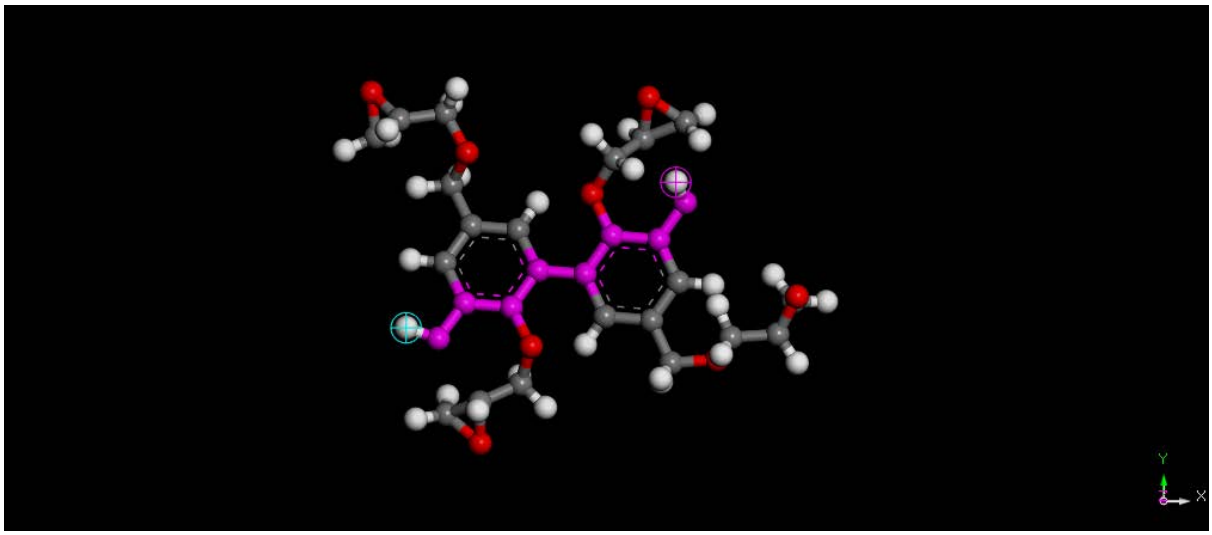

**Fig. 1.** TETRA-GEDVA monomer

## 2. Methodology

In present research work, molecular dynamics simulation has been performed using Material Studio software. MD is the most detailed molecular simulation method which computes the motions of individual molecules. Coupled Newton's equations of motion, which describe the positions and momenta, are solved for many particles in an isolated cluster or the bulk using periodic boundary conditions.

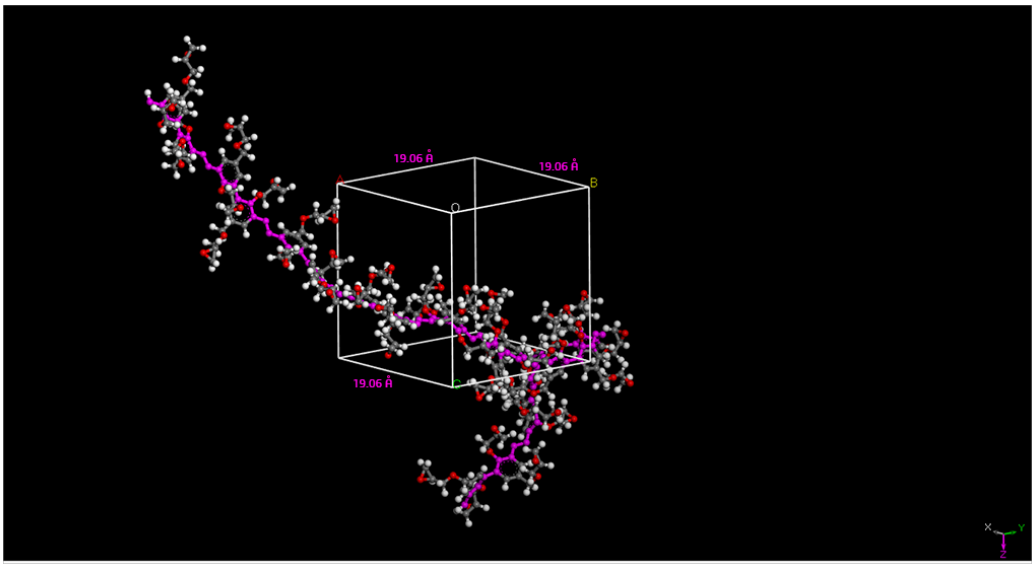


**Fig. 2.** Amorphous model of Tetra GEDVA

While building an amorphous cell the target density of cell was kept equivalent to the real density of the epoxy Tetra GEDVA i.e. 1.2 gm/cm$^3$. Table 1 shows the amorphous cell calculation parameters used for the present study. In densely packed amorphous cell 20 molecules of the triangular model have been used. Energy minimization and geometric optimization have been employed to stabilize the structure. Dynamic stability has been done using the Forcite module employing NPT ensembles. NPT is two commonly used ensemble

during MD simulation of biomolecules. NPT must be used during equilibration just before changing to a constant volume ensemble). The control parameters for the MD simulations on Forcite Dynamics has been shown in Table 2. The mechanical properties of the parameters are presented in Table 3. Furthermore, annealing has been performed using the NVT ensemble to keep volume and density intact. The dynamic run has been done followed by energy minimization and Investigation of mechanical properties of graphene reinforced epoxy nanocomposite using molecular dynamics 227 geometry optimization. The control parameters for Forcite Dynamics and Forcite Anneal.

Table 1. Amorphous cell calculation parameters

| Task | Construction |
|---|---|
| Density | 1.200g/cc |
| Optimize geometry | Yes |
| Number of frames | 1 |
| Loading steps | 1000 |
| Check ring spearing | Yes |
| Check close contacts | No |
| Check energies | Yes |
| Bias temperature | 298.000K |
| Look ahead | 1 |

Table 2. Control Parameters for MD Simulation (Forcite Dynamics)

| Force-field | COMPASS II |
|---|---|
| Temperature control | Berendsen |
| Pressure control | Berendsen |
| Initial velocity | Random |
| Temperature | 298K (25°C) |
| MD ensemble | NPT |
| Pressure | 0.3 GPa |
| Time step | 1 fs (femtosecond) |
| Duration of Simulation | 10 ps (pico second) |
| No. of steps | 20000 |
| Frame output rate | Per 1000 frames |

Table 3. Forcite Mechanical Properties

| **Energy parameters** | |
|---|---|
| Calculation method | Static |
| Forcefield | Compass |
| Charge | Forcefield assigned |
| **Vander waals terms** | |
| Summation method | Ewald |
| Accuracy | 0.001 kcl/mol |
| Buffer width | 0.5 A |
| Summation method | Atom based |
| Truncation method | Cubic spline |
| Cut off distance | 12.5 A |
| Spline width | 1A |
| Long range correction | Yes |
| Buffer width | 0.5A |

## 3. Results of Modelling and Simulation

The simulation has been done at room temperature i.e. 25 degrees centigrade (298 K) and external pressure was 0.3 GPa, which shows the temperature stability of the developed model with time. Figure 3 shows the Forcite Temperature Dynamics graph of epoxy. It shows that the temperature of the model increases and rose to room temperature. As the simulation proceeds, there is no change in the temperature profile which suggests that the model is dynamically stable. Using the control parameters as depicted in Table 1, the predicted density of the developed amorphous cell is 1.2 gm/cm$^3$, which is very close to the actual density of the epoxy TetraGEDVA at room temperature. Figure 4 shows the forcite dynamics energies for the amorphous cell of TetraGEDVA. Furthermore, the stability of the developed model has also confirmed the Forcite Dynamics energies trajectory as shown in Fig. 4. It shows that all the energies (potential energy, kinetic energy, non-bond energy, and total energy) are constant as the simulation progresses. Lower the kinetic energy more stable is the model which also confirms the thermal stability of the model. Figure 5 presents the amorphous cell of Graphene Reinforced Epoxy. The coordinates are also present in Fig. 5. The optimized structure is further used for creating graphene sheet reinforcement to obtain a graphene-based nanocomposite. A single layer graphene sheet (consisting of 70 atoms) has been randomly reinforced into the epoxy matrix. In the microscopic view, the nanoparticle reinforced Polymer Matrix composite is considered as the anisotropic material, while close to isotropic material on macro-level [16-17].

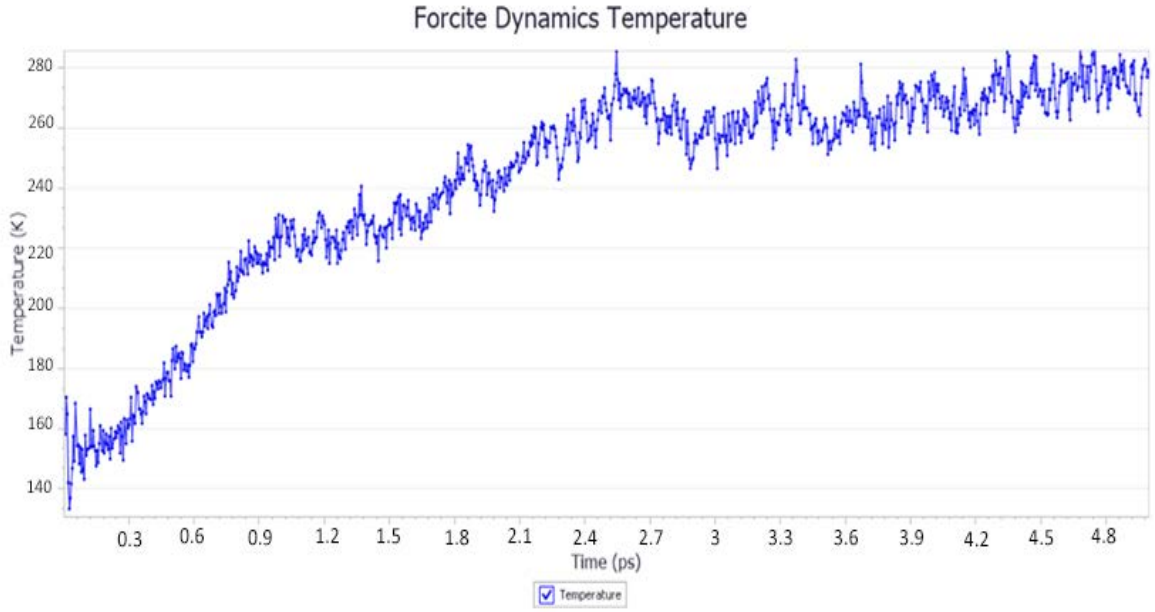


**Fig. 3.** Forcite Temperature Dynamics graph of epoxy

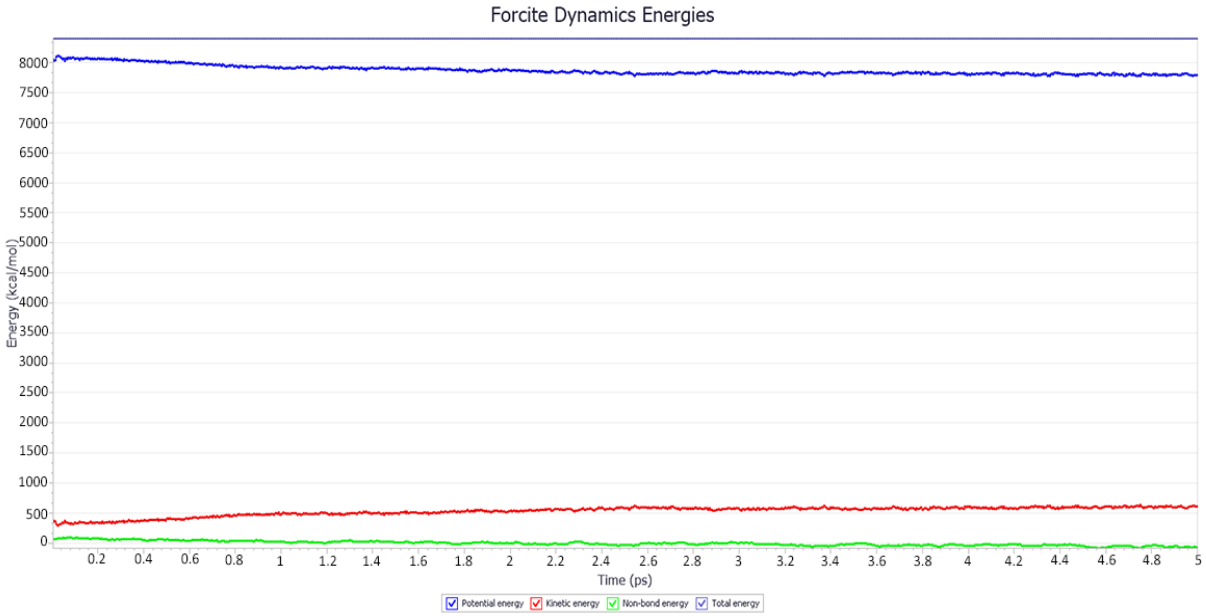


**Fig. 4.** Forcite Dynamics Energies for Amorphous cell of TetraGEDVA

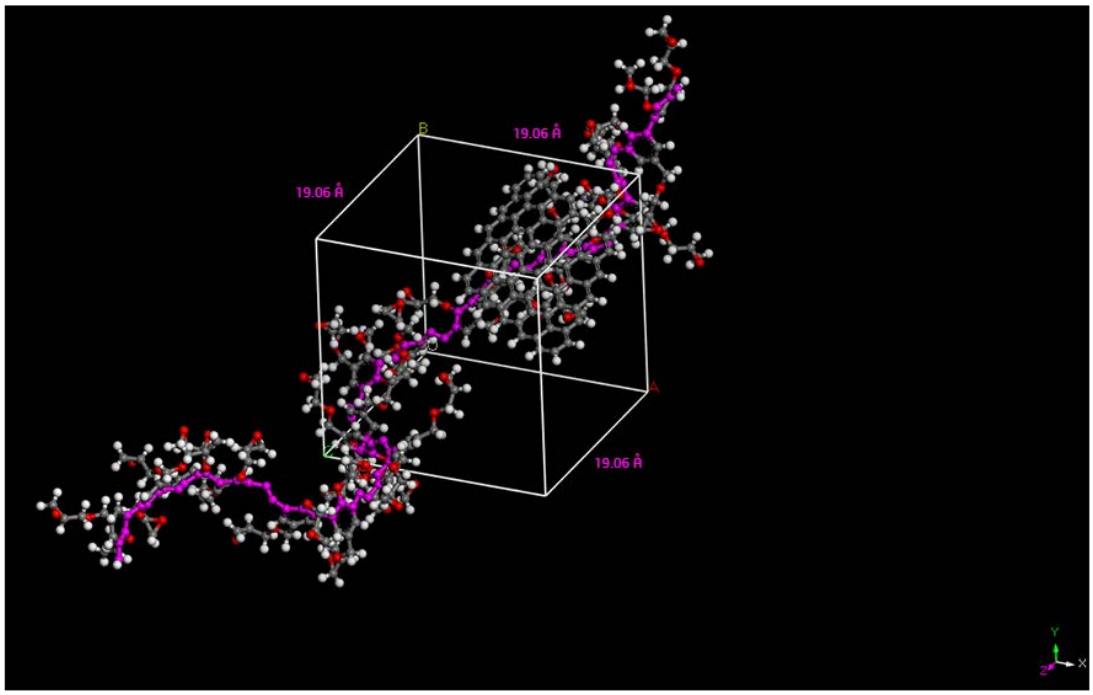


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**Fig. 5.** The amorphous cell of Graphene Reinforced Epoxy

In recent years, the MD simulation has already been applied in the study of materials on a certain scale with the rapid advancement of computer technology. Therefore, the MD simulation becomes an important method to predict the mechanical properties of polymeric materials [18]. The graphene sheet is a two-dimensional structure that consists of carbon atoms bonded by the hybridization of sp2 electrons. Single-layer graphene has very high mechanical properties. The mean Young's modulus of single layer zigzag graphene sheet with a length 20.18 nm and width 4.18 nm is 1.033 TPa.

Typically, graphene sheets are obtained from graphite oxide (GO). Hence, in the atomistic model, the carbon atoms at the edge of the graphene were kept terminated by adding hydrogen atoms.

## 4. Conclusion

MD simulation has been employed on two amorphous cell models. One model consists of cured TetraGEDVA and another model is obtained after reinforcement of a graphene sheet into the matrix of TetraGEDVA. The mechanical properties have been obtained after the Forcite dynamic simulation with constant strain minimization. Simulations using COMPASS force-field have been performed in the Forcite module. Youngs Modulus has been predicted using the Forcite Mechanical Properties module. The obtained mechanical properties are presented in Table 4 for Forcite Dynamics Energies for Amorphous cell of TetraGEDVA and Table 5 presents the obtained results for Youngs Modulus of the amorphous cell of Graphene Reinforced TetraGEDVAepoxy.The estimated amorphous cell density is 1.2 gm / $cm^3$, which is very close to the actual TetraGEDVA epoxy density at room temperature.

Table 4.Forcite Dynamics Energies for Amorphous cell of TetraGEDVA

| Young modulus (GPa) | Poision ratio |
|---|---|
| X=2.6122 | Exy=0.0550 Exz=0.4147 |
| Y=-3.0213 | Eyx= -1.0330 Eyz=-1.1483 |
| Z=8.0053 | Ezx=1.2708 Ezy=0.1875 |

Table 5. Youngs Modulus of amorphous cell of Graphene Reinforced TetraGEDVA epoxy

| Young modulus (GPa) | Poisson ratio |
|---|---|
| X=12.7491 | Exy=4.0107 Exz=0.1029 |
| Y=13.8048 | Eyx=4.3428 Eyz=-1.3534 |
| Z=3.3243 | Ezx= -0.0268 Ezy=0.3259 |

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