

**ONR Session**

**Molecular Dynamics Simulations of Graphite –Vinylester  
Nanocomposite and its Constituents**

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## ABSTRACT

Molecular dynamic simulations are used to simulate graphite-vinylester nanocomposites and their constituents. Simulation and geometrical parameters are studied to compare their effects on mechanical properties of matrix, reinforcement, interface, and composite. Young's modulus of 1.3 TPa for a single graphene layer and 1.16 TPa for the graphite are obtained. Interfacial shear strength is found to be 283 MPa for graphene, and 135 MPa for graphite. This paper shows that exfoliated Graphite nanoplatelet (xGnP) improves the elastic properties of vinylester-graphene nanocomposites.

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## INTRODUCTION

Nanolayer reinforcement of composite materials can greatly improve the material's structural and physical performances such as high stiffness, high heat deflection temperatures, low thermal expansion coefficients, high tensile strengths, and low permeation rates, without adding significant weight. For example, nanolayer polymer can achieve greater thermal stability (less flammable) with reduced permeability (improved barrier performance) [1-4]. Nanolayered reinforcements distribute internal stresses more uniformly by allowing greater dimensional latitude in the forming and shaping processes, as compared to conventional macroscale reinforcements. The unparalleled ability of clay nanolayers to boost mechanical properties of an engineering polymer (nylon-6) was first demonstrated by Toyota researchers. With only 4.2 wt % of clay nanolayers, the modulus doubled and heat distortion temperature increased by 80°C, compared to the pristine polymer, along with a reduction in permeability for water and an increase in flame retardant properties. A critical issue for the development of nanotechnology is our ability to understand, to model, and to simulate the behavior of the small structures and to make the connection between the nano structure properties and their macroscopic functions. Material modeling and simulation helps to understand the process, to set the objectives that could guide laboratory efforts, and to control material structures, properties, and processes at physical implementation. These capabilities are vital to engineering design at the component and systems level [5-10]. In general, nanoplatelet composites are classified into four types, conventional composite, intercalated composite, long range ordering composite (LRO) and disordered composite (Figure 1). In a conventional composite, clay or graphite exists as a layered material with layers held together by Van der Waals forces without any intercalation or exfoliation. Exfoliated graphene platelet are shown in Figure 2.a. The size of the platelet reinforcements is in the order of microns. In an intercalated composite Figure 2.b, polymer chains are introduced into the graphite galleries, but the graphite still retains its layered structure. The distance between layers is in the range of 10~30Å. The size of the layered graphite extends from several hundred nanometers (nm) to several microns. Exfoliated composites have exfoliated and dispersed graphite platelets with 1 nm thickness and several hundred-nm widths. This type can be divided into two groups, long-range ordered (LRO) (Figure 1.c) and disordered composites (Figure 1.d). LRO composites have intercalated separated graphite platelets within (30~105Å), so that the adjacent platelets cannot interact each other. This allows a comparable reinforcing effect to that of disordered composites. The key points of making platelet nanocomposites are: intercalation of polymers inside the galleries and exfoliation of platelets in the matrix. Exfoliation leads to the improvement of bulk reinforcement by increasing its mechanical properties and aspect ratio.

In order to understand nanocomposites, atomic structures, interfacial interaction between different matrices, and nanoreinforcements, atomic level interactions should be studied. Mechanical properties of nanocomposites could be predicted by realistic computational techniques that vary in time and length scales [11-13]. Molecular dynamics simulations can provide the structure and dynamic intercalated

molecules. It is used to model nano layered graphite polymeric nanocomposites and their constituents elastic properties. Molecular interactions are described by a forcefield. Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies (COMPASS) force field encounters for two function categories valence terms including the diagonal and off-diagonal cross coupling terms and nonbond interaction terms. The valence terms represent internal coordinates of bond, angle, torsion angle, and out-of-plane angle, and the cross coupling terms include two or three internal coordinates potentials. The nonbond interaction terms include Van der Waals for the Lenard-Johns function and a Coulombic function for electrostatic interactions [14]. This was performed using commercial software Material Studio 4.1 [15].

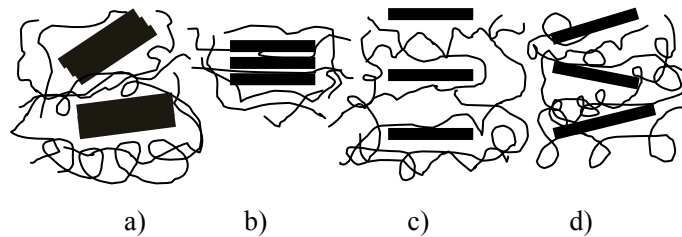


Figure 1. Schematic Diagram of Nanocomposites  
a) Conventional b) Intercalated c) Long Range d) Disordered

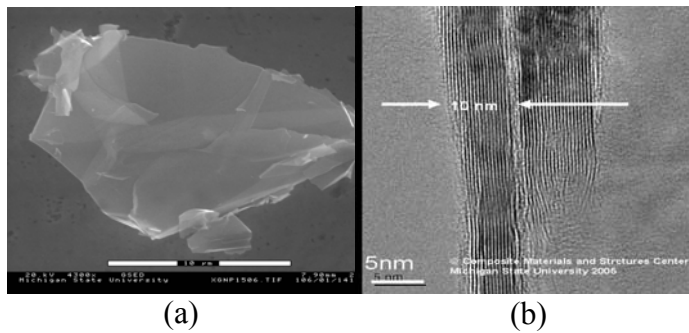


Figure 2. Images of xGnP: (a) SEM (Lateral view), (b) TEM (Edge view) (Courtesy of L. T. Drzal, 2009).

## **SIMULATION OF GRAPHENE PLATELET COMPOSITES USING MOLECULAR DYNAMICS**

### **Molecular Dynamic Simulations of Graphene/Graphite**

Graphene is a single layer  $sp^2$ -bonded carbon sheet forming a honeycomb crystal lattice [16], they were first introduced by Mouras, et al. (1987) as the two dimensional (2D) form of graphite. Novoselov et al. (1999) [17, 18] reported the 2D carbon material as the gigantic flat fullerene molecules and described their

electronic properties. A Young's modulus of 1.0 TPa, and intrinsic strength of 130 GPa were measured by nanoindentation atomic force microscope for the monolayer graphene sheet [19]. Those measurements had categorized the graphene monolayer sheet as the strongest material ever measured. Consequently, Graphene nanocomposites are expected to perform with extremely enhanced mechanical properties. Exfoliated Graphite Nano-Platelets (xGnP) are new types of nanoparticles that consist of graphene stacks that are 1-15 nm thick, with diameters ranging from sub- micrometer to 100 micrometers. xGnP share chemical structures with Carbon Nano Tubes (CNT), in fact their edges could be easily modified chemically for dispersion enhancement in polymeric composites [16].

Graphite atomic hexagonal crystal, group 186 P63MC is constructed with dimensions shown in Figure 3. Molecular dynamic geometry parameters such as periodic cell size and number of layers, are simulated to study their effect on graphene mechanical properties. NVT, which stands for constant Number of atoms, constant Volume, and constant Temperature, combined with Anderson thermostat is the thermodynamic ensemble that is applied through all the simulated configurations. COMPASS is the force field chosen for all molecular dynamics simulations [12, 13, 20].

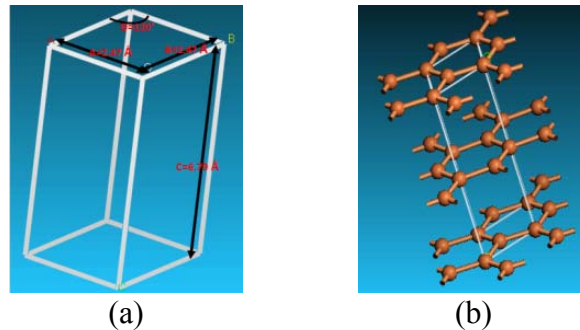


Figure 3. Molecular Graphite Crystal Dimensions

A structure energy minimization followed by a dynamic system equilibration under NVT ensemble is applied for a certain dynamic time. In which the dynamic time is proportional to the number of atoms included in the supercell simulated, 0.1 fs dynamic time step is kept constant for all graphene simulations and a 100 kcal/mol energy deviation.

## GRAPHENE MECHANICAL PROPERTIES

Graphene supercells of different sizes are shown in Figure 4. Elastic constants of the numerous super cells are shown in Table I. The periodic cell size for the graphene is a 2 supercell crystal.

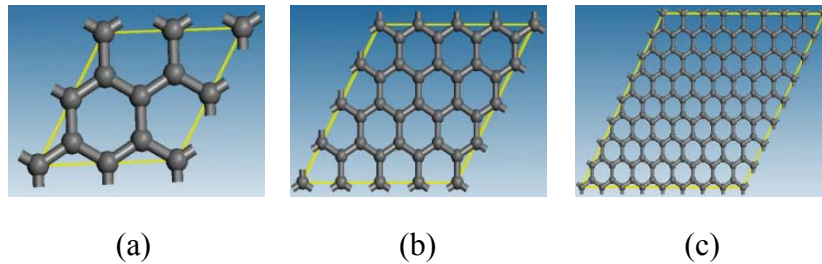


Figure 4. Graphene atomic super cell (a) Graphene Two Super Cells,(b) Graphene Four Super Cells, (c) Graphene Eight Super Cells.

TABLE I. GRAPHENE ENGINEERING CONSTANTS VERSUS NUMBER OF SUPERCELLS

Graphene Unit cell (NVT)				
Single Layer	Number of Supercells			
Eng. Constants	2*2 (8 atoms)	4*4 (32 atoms)	6*6 (70 atoms)	8*8 (128 atoms)
$E_{11}$ (GPa)	1373.3	1373.7	1373.9	1373.7
$E_{22}$ (GPa)	830.3	831.8	832.1	832.3
$\nu_{12}$	0.30	0.31	.31	.31
$M_{23}$ (GPa)	340.5	340.5	340.5	340.5
$K_{23}$ (GPa)	621.1	625.4	626.3	626.6

## GRAPHITE MECHANICAL PROPERTIES

Effect of Unit Cell Size:

Figure 5 shows a double layered graphite molecular supercell that was simulated to study the effect of supercell size for a graphite molecular structure.

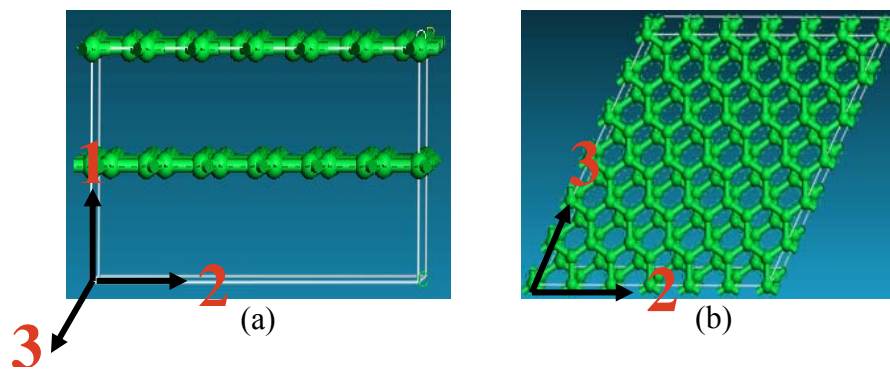


Figure 5. Double Layered Graphite Super Cell (a) Side view, (b) Top view.

Table II, and table III show the engineering constants for the graphite molecular structure of different supercell sizes. It has been shown from tables mentioned that the engineering constants tend to be constant for both supercell structures at 4\*4 size for the double wall, and a 8\*8 for the four layered graphite. Increasing the number of layers simulated requires a larger supercell to represent the periodic boundary cell.

TABLE II. DOUBLE LAYER GRAPHITE ENGINEERING CONSTANTS VERSUS NUMBER OF SUPERCELLS

Double Layer	Graphite (NVT) Number of Supercells				
	4*4 (64 atoms)	6*6 (144 atoms)	8*8 (256 atoms)	10*10 (400 atoms)	12*12 (576 atoms)
$E_{11}$ (GPa)	26.9	27.5	27.5	27.6	27.7
$E_{22}$ (GPa)	1159.6	1160.3	1160.3	1160.2	1160.2
$\nu_{13}$	0.0	0.0	0.0	0.0	0.0
$M_{23}$ (GPa)	406	406.2	406.2	406.2	406.1
$K_{23}$ (GPa)	1014	1014.8	1014.8	1015	1015

TABLE III. FOUR LAYER GRAPHITE ENGINEERING CONSTANTS VERSUS NUMBER OF CELLS

Graphene Unit cell (NVT)		
Four Layer	Number of Supercells	
Eng. Constants	8*8 (512 atoms)	12*12 (1152 atoms)
$E_{11}$ (GPa)	29.2	29.1
$E_{22}$ (GPa)	1161.3	1160.6
$\nu_{12}$	0.0	0.0
$M_{23}$ (GPa)	406.6	406.4
$K_{23}$ (GPa)	1015.4	1014.7

Effect of Number of Layers:

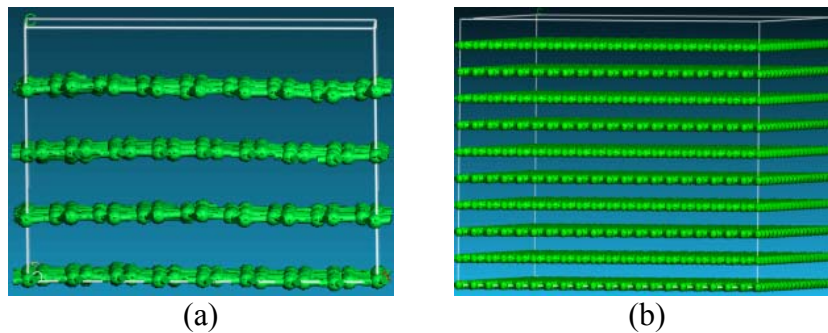


Figure 6. Multi Layered Graphite Super Cell: (a) Four Layer, (b) Ten Layer

Number of layers simulated to study the geometrical effect on the graphite mechanical properties. Figure 6 shows a molecular crystal structure for a four layered and a ten layered graphite supercell. Table IV shows the engineering constants for a double, four, and a ten layered graphite periodic cells, the variation of the engineering constants for the multi layered graphite periodic cells was less than 5%.

TABLE IV. PERIODIC GRAPHITE CELLS ENGINEERING CONSTANTS VERSUS NUMBER OF WALLS

Graphite Unit cell (NVT)			
Number of Layers			
Eng. Constants	2 Layers (576 atoms)	4 Layers (512 atoms)	10 Layers (9640 atoms)
$E_{11}$ (GPa)	27.7	29.2	27.8
$E_{22}$ (GPa)	1160.2	1161.3	1160.1
$\nu_{12}$	0.0	0.0	0.0
$M_{23}$ (GPa)	406.1	406.6	406.05
$K_{23}$ (GPa)	1015	1015.4	1015

### Molecular Dynamic Simulations of Vinylester

DERAKANE 411-350 Epoxy Vinyl Ester Resin is a copolymer thermoset resin which is produced by the esterification of an epoxy resin with unsaturated monocarboxylic acid. The reaction product is then dissolved in a reactive solvent, such as styrene, to (35-45) percent content by weight. It can be used as an alternative to polyester and epoxy materials in matrix or composite materials, where its characteristics, strength, and bulk cost intermediate between polyester and epoxy. Vinylester has low resin viscosity, less than polyester and epoxy [16]. Epoxy

based vinylester has remarkable corrosion resistance, physical properties, and improved adhesion compared to polyesters. That is due to their chemical composition, and the presence of polar hydroxyl and ether groups.

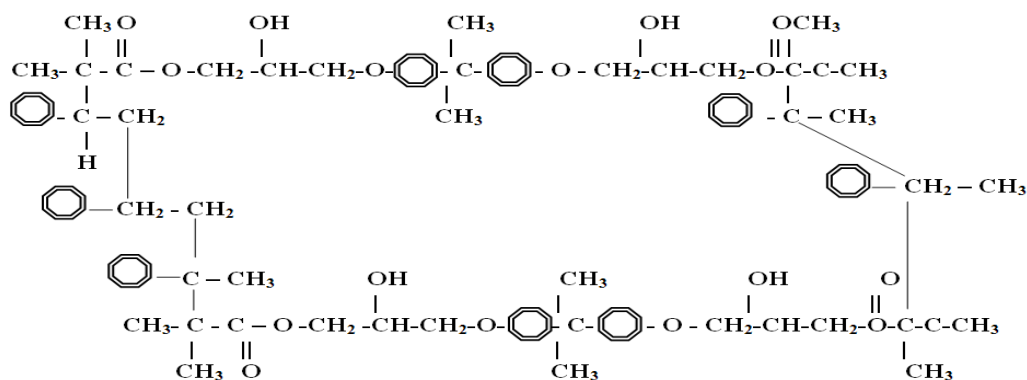


Figure 7. Single VE Chain: 35% Styrene, 65% Epoxy

Vinylester simulated chains are 65% epoxy, 35% styrene; Figure 7 shows a schematic chemical chain. Glass transition temperature ( $T_g$ ), is the temperature at which the amorphous polymer is converted between rubbery and glassy states, it is considered the most important mechanical property for all polymers, due to the fact that some physical properties undergo a drastic change under different glass transition temperature, such as hardness, Young's module, and volume.

Amorphous cell molecular dynamics model is recommended for amorphous polymers to optimize their mechanical behavior, surface, and interface interactions. It is a suite of computational tools that allow assembly of representative models of complex amorphous systems, and anticipate the key properties. Simulation parameters are set which include system composition, temperature and density. Periodic bulk disordered systems containing selected vinylester chain molecules in realistic equilibrated conformations are the selected force field COMPASS. Each amorphous cell is carried through a series of energy minimizations by conjugate gradient method, and canonical dynamic thermodynamic equilibration at room temperature at 1fs rate. A single vinylester chain of 320 atoms (Figure 8a), is repeated with an equilibrated conformational order in a periodic bulk cell. Several Amorphous cells are constructed with 8, 10, and 12 random confirmations of vinylester chains (Figure 8b). Vinylester bulk periodic cell density is 1.04 gm/cm<sup>3</sup> at room temperature 298K, and  $T_g = 400$  K [21, 22]. Periodic polymeric cells temperature is raised beyond  $T_g$ , and cooled back to room temperature. Static mechanical properties are calculated for each equilibrated cell [12, 13].

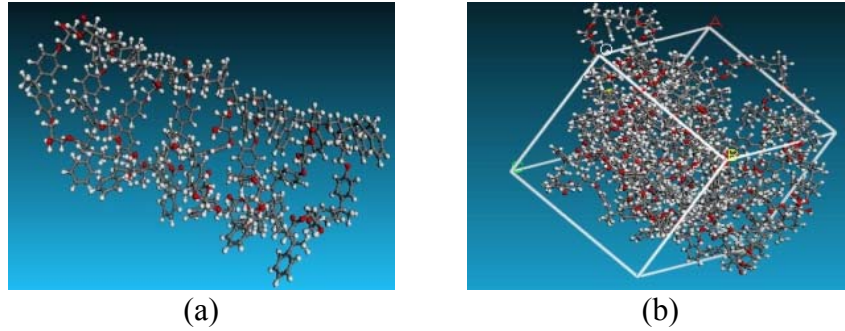


Figure 8.a) Atomic vinyl ester Single Vinyl ester Chain (230) Atoms b) 10 Chain Vinyl ester Unit Cell (2300) Atoms

Table V shows the engineering constants for a vinyl ester amorphous cell, for 6, 10, and 12 chains. From results shown, an amorphous cell of 10 chains of vinyl ester with a 3200 total number of atoms is the periodic cell of such a polymeric structure, engineering constants didn't vary between the 10 and the 12 amorphous cells.

TABLE V. VINYLESTER ENGINEERING CONSTANTS VERSUS NUMBER OF CHAINS

Eng. Constants	6 Chains	10 Chains	12 Chains
E11 (GPa)	2.83	3.7	3.7
$\nu_{12}$ (GPa)	0.30	0.31	0.31
M23 (GPa)	1.08	1.407	1.407
K23 (GPa)	2.8	3.37	3.37

### Molecular Dynamic Simulations of Graphene Vinyl ester Interfacial Properties

Nanocomposites are known for their high surface/volume ratio, small volume fraction of fillers will induce high strength composites. a key role of those high performance material is the interfacial strength between the nanoreinforcements and polymeric chains. Weak interfacial strength will induce low stiffness and strength. High interfacial strength will result high stiffness, strength, and toughness composite [23]. Molecular dynamic simulations can provide detailed information on interface structure and interaction. According to Gou et al. [24], the pullout energy,  $E_{pull-out}$ , is defined as the energy difference between the fully embedded graphene plate and the complete pull-out configuration. It can be related to the interfacial shear stress,  $\tau_i$ , by the following relation:

$$E_{pullout} = \int_0^L 2(W+t).(L-x)dx = (W+t)L^2 \quad (1)$$

$$\tau_i = \frac{E_{pullout}}{(W+t)L^2} \quad (2)$$

where,  $W$  and  $L$ ,  $t$  are the width, length, and thickness of the graphene plate, respectively, and  $x$  is the displacement of the graphene sheet.

The  $E_{pull-out}$  for the vinylester graphene 149.61 kcal/mol., energy plot is shown in figure 11(a). The properties of the unit cell simulated for the pull-out energy is: density of 0.37 gm/cm<sup>3</sup>, molecular weight of 10672 gm/mol, and cell dimensions of (L=29.64Å, W=29.64Å, t=3.4Å). According to equation 2,  $\tau_i = 283$  MPa, which is double the interfacial strength of the SWCNT- Polyethylene reported in [25, 12]

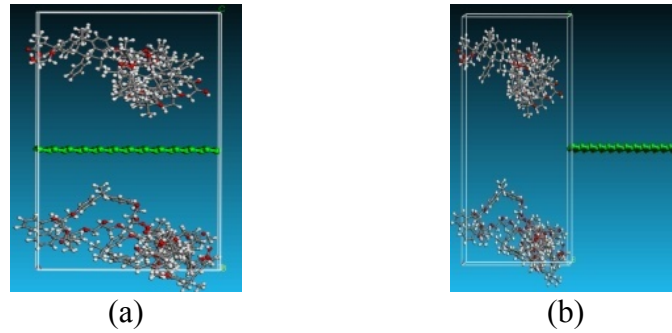


Figure 9. Atomic Model For Graphene Reinforcement Interfacial Pull-out

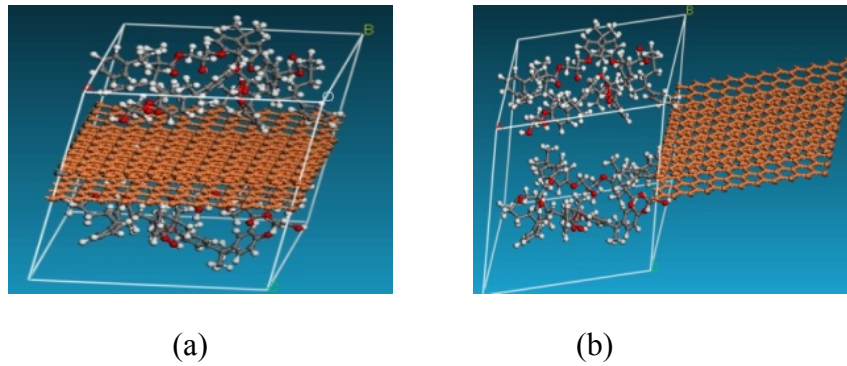


Figure 10. Atomic Model For Graphite Reinforcement Interfacial Pull-out

A similar atomic cell structure was constructed for the graphite (Figure 10) to study the interfacial strength of a multi layered graphene nanoplatelet. Double layered graphite was chosen with a density of 0.572 gm/cm<sup>3</sup>, molecular weight of 14128 gm/mol, and cell dimensions of (L=29.64Å, W=29.64Å, t=3.4Å).  $E_{pull-out}$  for

the double layer of graphite is 69.8k-cal/mole figure 11(b). The interfacial strength calculated from equation 1-2 is 135.13 MPa, which is less than half graphene interfacial strength.  $\tau_i = 135$  MPa. Interfacial strengths summary are shown in table V.

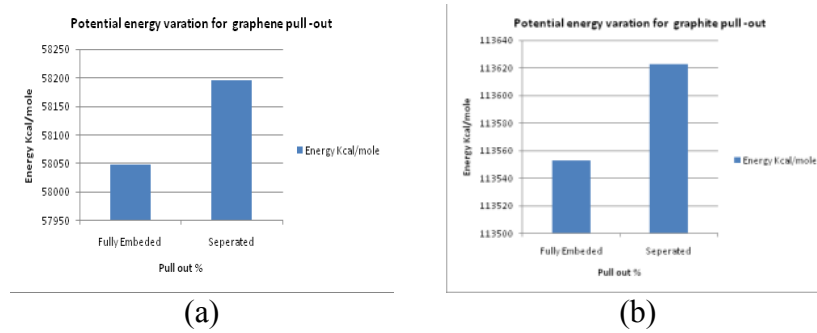


Figure 11. Potential Energy Variation For a Pull-out Test From Vinylester Matrix Composite: (a) Graphene, (b) Graphite

TABLE VI. INTERFACIAL STRENGTH FOR VINYLESTER GRAPHENE AND GRAPHITE COMPOSITES

Composite	Interfacial Strength ( MPa)
SWCNT -Polyethylene	133
Graphene - Vinylester	283
Graphite -Vinylester	135

### Molecular Dynamic Simulations of Graphene Composites

Molecular dynamic simulations are carried out for the graphite – vinylester, and exfoliated graphene –vinylester composites. The simulation conditions and cell sizes that have been constructed are mentioned in Table VI. The two step NVT simulation described earlier in matrix molecular modeling are applied to the composite cases too. The temperature of the system is maintained at 298K throughout the simulation.

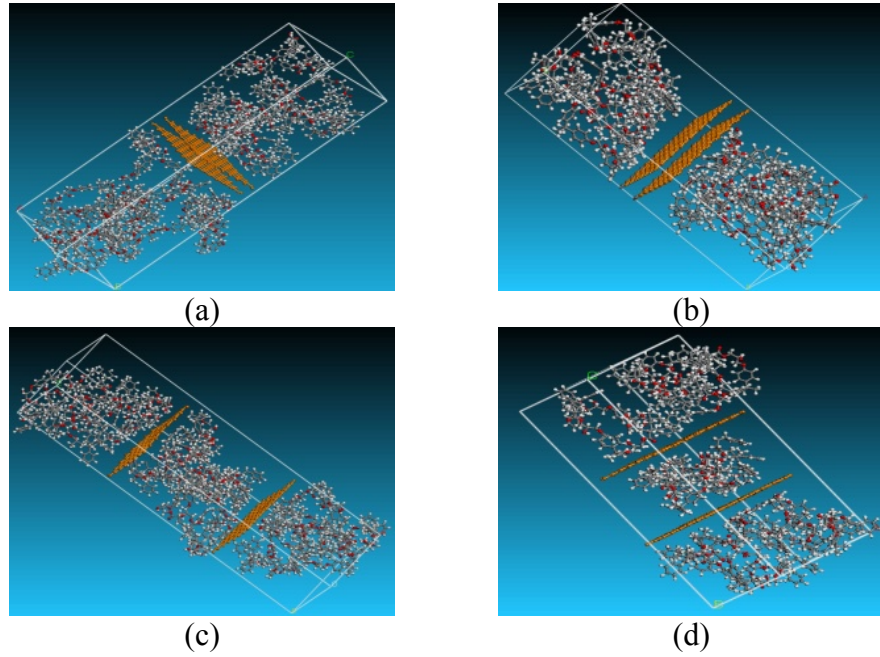


Figure 12. a) 10%Graphene Vinyl ester Composite, (b) 20%Graphene Vinyl ester Composite, (c) 10% Exfoliated Graphene Vinyl ester Composite, (d) 20% Exfoliated Graphene Vinyl ester Composite.

Stiffness matrices for 10 and 20 weight percentage reinforcements are shown in table 6 for different simulation conditions. Results show that exfoliated graphene platelets have higher elastic properties than the graphite composites.

TABLE VII. GNP VINYLESTER COMPOSITES STIFFNESS MATRICES

GnP -Vinylester Composite Stiffness Matrix: 10%	
Unit Cell size: (19.76*19.76*58.6) A	
Triclinic cell: $\alpha=\beta=90^\circ, \gamma=90^\circ$	
Thermodynamic: NVT	
Number of Atoms: 2232	
Temperature: 400K	
Elastic Properties: at 298K	
$C_{ij} = \begin{bmatrix} 5.9 & 1 & 1.8 & 0 & 1.9 & 0 \\ 3.3 & 147 & 34.2 & 0 & 0 & 88.7 \\ 3.9 & 35.7 & 142.5 & 0 & 0 & 88.3 \\ 0 & 0 & 0 & 15.2 & 13.9 & 0 \\ 0 & 0 & 0 & 13.3 & 15.1 & 0 \\ 0 & 87.7 & 89 & 0 & 0 & 94.5 \end{bmatrix}$	GPa

GnP -Vinylester Composite Stiffness Matrix: 20%

Unit Cell size: (19.76\*19.76\*91.54) A

Cubic cell:  $\alpha=\beta=90^\circ$ ,  $\gamma=90^\circ$

Thermodynamic: NVT

Number of Atoms: 3246

Elastic Properties: at 298K

$$C_{ij} = \begin{bmatrix} 3.2 & 1.5 & 2.50 & 0 & 0 & 0 \\ 1.8 & 228 & 56.8 & 0 & 0 & 137 \\ 1.3 & 57.6 & 229.5 & 0 & 0 & 139 \\ 1.3 & 57.6 & 229.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 20.3 & 20.9 & 0 \\ 0 & 139 & 139.9 & 0 & 0 & 143.2 \end{bmatrix} \text{ GPa}$$

xGnP -Vinylester Composite Stiffness Matrix: 10%

Unit Cell size: (19.76\*19.76\*58.6) A

Triclinic cell:  $\alpha=\beta=90^\circ$ ,  $\gamma=90^\circ$

Thermodynamic: NVT

Number of Atoms: 2232

Temperature: 400K

Elastic Properties: at 298K

$$C_{ij} = \begin{bmatrix} 18.4 & 9.3 & 7.2 & 0 & 0 & 0 \\ 6.7 & 135.9 & 52.4 & 0 & 0 & 0 \\ 8.1 & 63.7 & 129.2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 11.7 & 0 & 0 \\ 0 & 0 & 0 & 0 & 7.9 & 0 \\ 0 & 0 & 0 & 0 & 0 & 37.7 \end{bmatrix} \text{ GPa}$$

xGnP -Vinylester Composite Stiffness Matrix: 20%

Unit Cell size: (19.76\*19.76\*91.54) A

Cubic cell:  $\alpha=\beta=90^\circ$ ,  $\gamma=90^\circ$

Thermodynamic: NVT

Number of Atoms: 3246

Elastic Properties: at 298K

$$C_{ij} = \begin{bmatrix} 4 & 1.4 & 3.2 & 0 & 0 & 0 \\ 2.1 & 230 & 57.7 & 0 & 0 & 140.6 \\ 1.6 & 59.7 & 230.3 & 0 & 0 & 140 \\ 0 & 0 & 0 & 20.6 & 22.02 & 0 \\ 0 & 0 & 0 & 20.7 & 22 & 0 \\ 0 & 139 & 140 & 0 & 0 & 142.1 \end{bmatrix} \text{ GPa}$$

## CONCLUSIONS

Molecular dynamics simulations was used to estimate mechanical properties of nano composites made of graphite nano platelets and DERAKANE 411-350 epoxy vinyl ester resin. Young's modulus of 1.3 TPa was estimated for graphene layer. Elastic properties obtained for graphite were  $E_{11}=0.27$  TPa, and  $E_{22}=1.2$  TPa. Number of layers didn't affect the elastic properties for the multi layered graphite periodic cell. Interfacial strength for the graphene came out to be double the interfacial strength of the double layered of graphite. Exfoliated graphene nano platelet composite simulations show improved mechanical properties than the graphite sheets.

## ACKNOWLEDGMENT

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## REFERENCES

- [1] Lan, T. T., Kaviratna, P. D., Pinnavaia, T. J. 1995. "Mechanism of clay tactoid exfoliation in nanocomposites," *Journal of Chemistry of Materials*,7(11): 2144-2148.
- [2] Lan, T. T., Pinnavaia, T. J. 1996. "Clay-reinforced epoxy nanocomposites" *Mat. Res. Soc. Symp. Proc.* 435:79-84.
- [3] Vaia, R. A., Price, G., Ruth, P. N., Nguyen, H. T., Lichtenhan, J. 1999. "Polymer/layered silicate nanocomposites as high performance ablative materials," *Applied clay science*, 15(1): 67-92.
- [4] LeBaron, P. C., Wang, Z., Pinnavaia, T. J. 1999. "Polymer -Layered silicate nanocomposites," *Applied Clay Science*, 15(1):11-29.
- [5] Varley, R., J., Groth, A., M., Leong, K., H. 2007. "The role of nanodispersion on the fire performance of organoclay-polyamide nanocomposites," *Composite Science and Technology*, 68:2882-2891.
- Meyer, J. C., Geim, A. K., Kastnelson, M. I., Novoselov, K. S., Booth, T. J., Roth, S. 2007. "The structure of suspended graphene sheets," *Nature*,446:60

- [6] Figiel, L., Buckley, C. P. 2008. "Elastic constants for an intercalated layered silicates using the effective particle concept- A parametric and analytical continuum approaches," Computational materials science, in press.
- [7] Valavala, P.K., Odegard, G.M. 2008. "Thermodynamically-consistent multiscale constitutive modeling of glassy polymer materials," IUTAM Symposium on Modelling Nanomaterials and Nanosystems Proceedings of the IUTAM Symposium, Aalborg, Denmark, 19–22.
- [8] Zeng, Q. H., Yu, A. B., Lu, G. Q. 2007. "Multiscale modeling and simulation of polymer nanocomposites," Progress in Polymer Science, 2007, 33:191-269.
- [9] Harkin- Jones, Figiel, Spencer, Abu-Zurayk, Al-Shabib, Chan, Rajeev, Soon, Buckley, et al. 2008. "Performance enhancement of polymer nanocomposites via Multiscale modelling processing and properties," Plastics, Rubber & Composites, 37(2) 113- 125
- [10] Xiao, M., Sun, L., Liu, J., Li, Y., Gong, K. 2001. "Synthesis and properties of polystyrene/graphite nanocomposites," Polymer, 43:2245-2248.
- [11] Leach, R. A., 2001. "Molecular Modelling Principles and Application," Pearson Education, EMA.
- [12] Al-Ostaz A., Pal G. 2008. Molecular dynamics simulation of SWCN-polymer nanocomposite and its constituents, Journal of Materials Science, 2008, 43:164-173.
- [13] Alkhateb H., Al-Ostaz A. 2009. "Geometric and simulation parameter effects on elastic moduli of multi-walled carbon nanotubes using molecular dynamics approach," Submitted to Journal of Materials Science.
- [14] Sun H. 1998. "COMPASS: An ab initio Forcefield Optimized for condensed-Phase Application Overview with details on Alkane and Benzene Compounds," Journal of Physical Chemistry B, 102: 7338.
- [15] MS Modeling 4.0 Online Help Manual, Accelrys Inc., 2005.
- [16] Wikipedia
- [17] Novoselov, A. K., Geim, A. K., Morozov, S. V., Jaing, D., Zhang, Y., Dubonus, S. V., Grigrieva, I.V., Firsov, A. A. 2004. "Electric field in atomically thin carbon films," Science, Oct 22
- [18] Novoselov, K. S., Jaing, D., Booth, T. J., Khotkevich, V. V., Morzov, S. V., Geim, A. K. 2005. "Two-dimensional atomic crystals," PNAS, 102(30):10451-10453.
- [19] Lee, C., Wei, X., Kysar, J. W., Hone, J. 2008. "Measurement of the elastic properties and intrinsic strength of monolayer Graphene," Science, 321:385- 388.
- [20] Anderson, H. C. 1980 "Molecular dynamics simulations at constant pressure and/or temperature," J. Chem. Phys., 72:2384.
- [21] Karger-Kocsis, J., Gryshchuk, O., Schmitt, S. 2003. "Vinylester /epoxy-based thermosets of interpenetrating network structure: an atomic force microscopic study," Journal of Materials Science, 38(3):413-420
- [22] Derkane Momentum <sup>TM</sup> 640-900. 2004. Epoxy Vinyl Ester Resin.

- [23] Wagner, H. D., Vaia, R. A. 2004 "Nanocomposites issues at the interface," *Materials Today*, 38-24.
- [24] Gou, J., Minaie, B., Wang, B., Liang, Z., Zhang, C. 2004. "Computational and experimental study of interfacial bonding of single-walled nanotube reinforced composites," *Computational Materials Science*,31:225-236.
- [25] Liao K, Li, S. 2001. "Interfacial characteristics of a carbon nanotube-polystyrene composite system" *Applied Physics Letters*, 79 (25):4225-4227.