

MOLECULAR DYNAMICS SIMULATIONS OF GRAPHITE – VINYLESTER NANOCOMPOSITES AND THEIR CONSTITUENTS

H. Alkhateb, A. Al-Ostaz, A.H-D. Cheng

Nano Infra Structure Group

The University of Mississippi, University, MS, 38677

ABSTRACT

The effects of geometrical parameters on mechanical properties of graphite-vinylester nanocomposites and their constituents (matrix, reinforcement and interface) are studied using molecular dynamics (MD) simulations. Young's moduli of 1.3 TPa and 1.16 TPa are obtained for graphene layer and for graphite layers respectively. Interfacial shear strength resulting from the molecular dynamic (MD) simulations for graphene is found to be 256 MPa compared to 126 MPa for graphite. MD simulations prove that exfoliation improves mechanical properties of graphite nanoplatelet vinylester nanocomposites. Also, the effects of bromination on the mechanical properties of vinylester and interfacial strength of the graphene–brominated vinylester nanocomposites are investigated. MD simulation revealed that, although there is minimal effect of bromination on mechanical properties of pure vinylester, bromination tends to enhance interfacial shear strength between graphite and vinylester in a considerable magnitude.

INTRODUCTION

A critical issue for the development of nanotechnology is the ability to understand, to model, and to simulate the behavior of these nano structures and to make the connection between nano structure properties and their macroscopic functions. Material modeling and simulation aid in understanding this process, help in setting objectives that guide laboratory investigation, and assist in setting controls on material structures, properties, and processes for physical implementation. These capabilities are vital to engineering design at the component and systems levels [5-10].

Nanolayer reinforcement of composite materials can greatly improve these material's structural and physical performance, such as stiffness, heat deflection

temperatures, tensile strengths. It also tends to lower thermal expansion coefficient and permeation rate without adding significant weight, thereby allowing nanolayer polymers to achieve greater thermal stability (to become less flammable) and to reduce permeability (improve barrier performance) [1-4]. Nanolayer-enhanced polymers distribute internal stresses more uniformly by allowing greater dimensional latitude during the forming and shaping processes, as compared to conventional macroscale reinforcements. For example, the unparalleled ability of clay nanolayers to boost mechanical properties of an engineering polymer (nylon-6) was first demonstrated by Toyota researchers. An increase of only 4.2 wt % of clay nanolayers doubled the modulus, increased heat distortion temperatures by 80 degrees C (compared to pristine polymer), reduced permeability for water, and increased flame retardant properties.

Carbon-based nanomaterials have been attracting much attention during the last decade, because of their superior mechanical, electrical and thermal properties. Since the late 1990's, research has been reported that intercalated, expanded, and/or exfoliated graphite nanoplatelets could also be used as nano-reinforcements in polymer systems. The key point of utilizing graphite as a nano-reinforcement is in its ability to be exfoliate into platelets of nanometer dimensions using Graphite Intercalated Compounds (GICs). Natural graphite is abundant and its cost is low compared to the other nano size carbon materials. The graphite nanoplatelets are expected to be marketed at approximately \$10-20/lb once high demand and full production is achieved. This is significantly less expensive than single wall nanotubes (SWNT) (>\$45,000/lb) or vapor grown carbon fiber (VGCF) (\$40-50/lb), yet the mechanical, electrical, and thermal properties of crystalline graphite flakes are comparable to those of SWNT and VGCF.

Graphene is a single layer sp^2 -bonded carbon sheet forming a honeycomb crystal lattice [11], first introduced by Mouras, et al. (1987) as the two dimensional (2D) form of graphite. Novoselov et al. (1999) [12, 13] reported that these 2D carbon materials formed gigantic flat fullerene molecules and first described their electronic properties. Lee et al. reported a Young's modulus of 1.0 TPa, and an intrinsic strength of 130 GPa measured by nanoindentation atomic force microscope for the monolayer graphene sheet [14]. By those measurements, Lee categorized the graphene monolayer sheet as the strongest material ever measured. Consequently, Graphene nanocomposites are expected to perform extremely enhanced mechanical properties. Exfoliated Graphite Nano-Platelets (xGnP) are new types of nanoparticles consisting of graphene stacks that are 1-15 nm

thick and 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 [15]. Figure 1 shows the morphology of xGnP. These nanoplatelets are typically less than 5 nm thick and can be synthesized with lateral dimensions ranging from less than 1 micron to up to 100 microns. The use of exfoliated graphite flakes (xGnP) opens up many new applications where electromagnetic shielding, electrical conductivity, high thermal conductivity, gas barrier resistance, high fracture toughness, or low flammability are required.

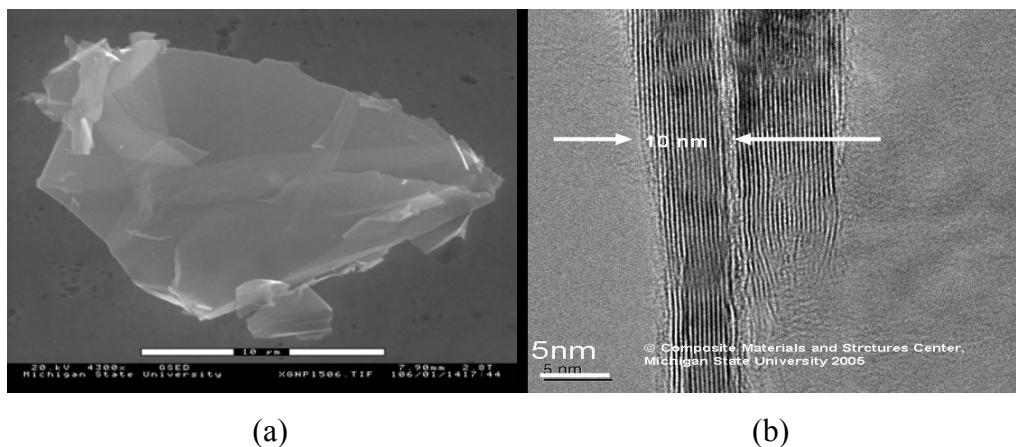


Figure 1. Images of xGnP: (a) Lateral view using SEM, (b) Edge view using TEM micrograph (Courtesy of L. T. Drzl).

Vinylester is a copolymer thermoset resin 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. Vinylester can be used as an alternative to polyester and epoxy materials in matrix or composite material because its distinctive characteristics, strength, and bulk cost lie intermediately between polyester and epoxy. Vinylester has low resin viscosity, less than polyester and epoxy [15,16], but the epoxy-based vinylester has remarkable corrosion resistance, physical properties, and improved adhesion compared to polyester due to their chemical composition, and the presence of polar hydroxyl and ether groups. Simulated vinylester chains are 65% epoxy and 35% styrene; Figure 2 shows a schematic vinylester chemical chain.

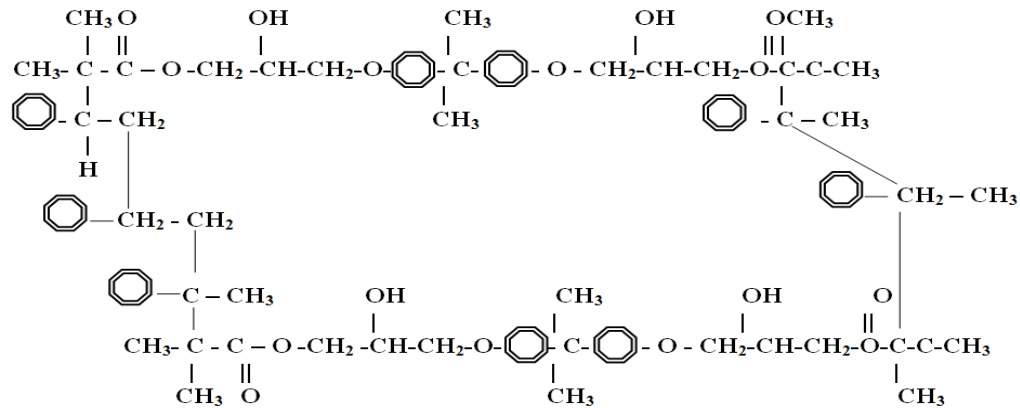


Figure 2. Single VE Chain: 35% Styrene, 65% Epoxy

Vinylester-resin systems have other challenge: poor resistance to crack propagation, brittleness, and large shrinkage that occurs during polymerization. Methods of incorporating nanoparticles into polymer matrices could be ex-situ, like dispersion of the synthesized nanoparticles into resin solution, or in-situ, like monomer polymerization process in the presence of the nanoparticles.

The interactions between the nanoparticles and the matrix for the ex-situ fabricated composites are normally van der Waals force; however, the in-situ synthesis methods may create strong chemical bonding within the composite. Introducing good interfacial bonding between nanofillers and the resin is often used to alleviate volume shrinkage, void formation and improve surface dispersion along with toughness. Control of interfacial adhesion appears to be crucial since a major cause of impact-related problems is believed to be associated with the level of adhesion at the interface between fiber and matrix. A variety of fiber surface treatment and modification techniques are used to control the interfacial bonding. The strong interface favors a brittle fracture mode with relatively low energy absorption; whereas, a weak interface favors a multiple shear mode with high energy absorption. Therefore, optimization of the interfacial adhesion is required to obtain excellent interfacial strength along with enhanced impact properties [16]. According to Gou, et al. [17], molecular dynamic simulations can provide detailed information on interface structure and interaction. The Vinylester bromination effect is simulated to study the effect of bromination on the interfacial strength of vinylester/graphene and vinylester/graphite nanocomposites. High interfacial strength

will result high stiffness, strength, and toughness in the composite [18,19]. Figure 3 shows a schematic chemical chain for a brominated vinylester.

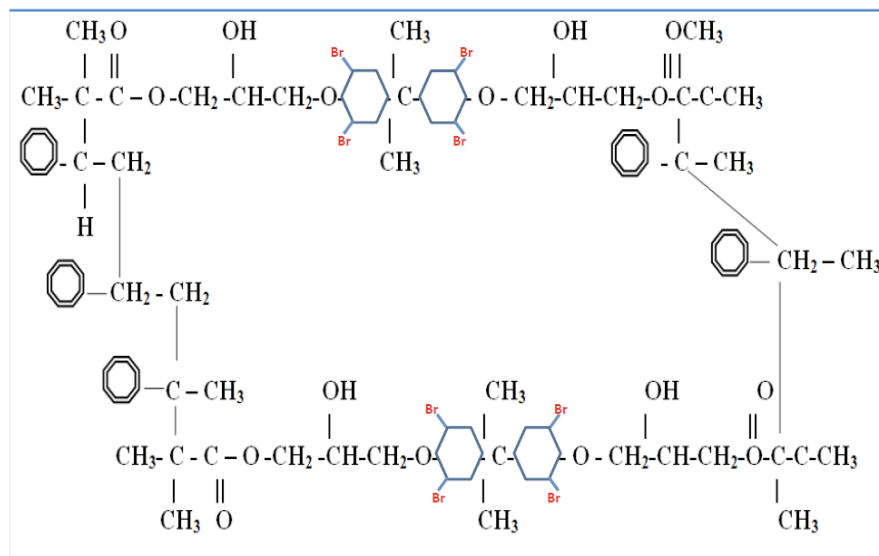


Figure 3. Molecular Structure of Brominated Vinylester

In general nanoplatelet composites are classified into four types: conventional composite, intercalated composite, long range ordering composite (LRO), and disordered composite (Figure 4). In a conventional composite (Figure 4a), clay or graphite exists as a layered material with layers held together by van der Waals forces without any intercalation or exfoliation. In an intercalated composite (Figure 4b), 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 both exfoliated and dispersed graphite platelets with 1 nm thicknesses and several hundred-nm widths. This type can be divided into two groups, long-range ordered (LRO) (Figure 4c) and disordered composites (Figure 4d). LRO composites have intercalated separated graphite platelets within (30~105Å) so that the adjacent platelets do not interact with each other. This configuration allows a comparable reinforcing effect for disordered composites. The key reasoning behind 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

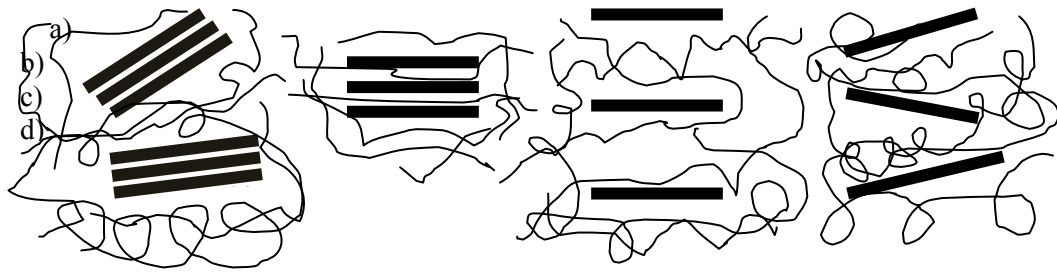


Figure 4. Schematic Diagram of Nanocomposites: a) Conventional, b) Intercalated, c) Long Range, and d) Disordered

In order to understand nanocomposites; atomic structures; interfacial interaction between different matrices; and nanoreinforcements; atomic level interactions should be studied in details. Mechanical properties of nanocomposites could be predicted by realistic computational techniques that vary in time and length scales [20-22]. Molecular dynamics (MD) simulations can provide the structure, and the dynamic intercalated molecules could provide MD is used to model nano layered graphite polymeric nanocomposites and their constituents elastic properties. After MD simulation is performed, the resulting deformed molecular structure is analyzed to determine the elastic constants. Following the initial stage, three tensile and three pure shear strains with magnitudes of ± 0.0005 are applied to the energy minimized system, with the system re-minimized following each deformation [23].

In the work presented in this paper, molecular interactions are described by Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies (COMPASS) forcefield. COMPASS force field accounts 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. The cross coupling terms include two or three internal coordinates potentials. The nonbond interaction terms include Van der Waals for the Lennard-Jones function, and a Coulombic function for electrostatic interactions [24]. The MD simulations are performed using commercial software, Material Studio 4.1 [23].

SIMULATION OF GRAPHENE PLATELET COMPOSITES USING MOLECULAR DYNAMICS

Simulations of Graphene/Graphite

Graphite atomic hexagonal crystal group 186 P63MC is constructed with dimensions shown in Figure 5. 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, associated with Anderson thermostat is the thermodynamic ensemble applied through the entire simulated configurations.

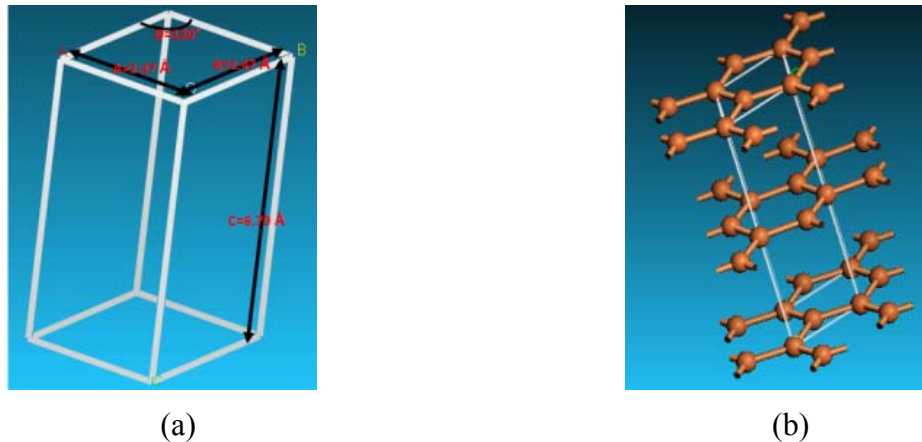


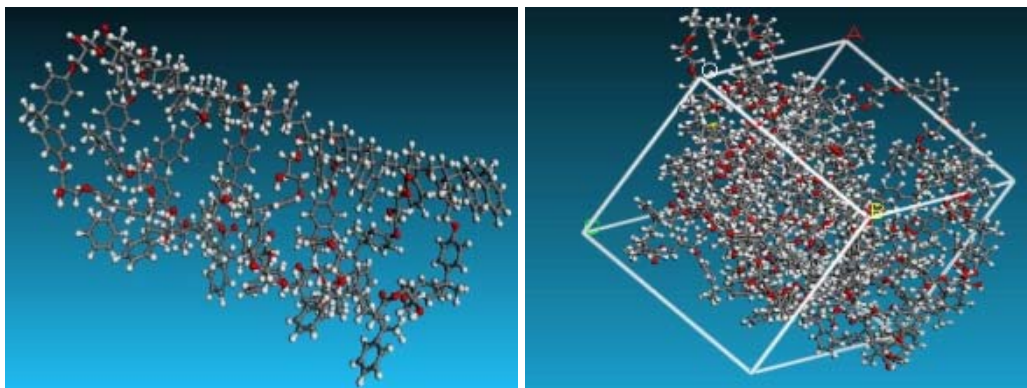
Figure 5. Molecular Graphite: (a) Crystal dimensions, (b) Atomic crystal structure

A structure energy minimization followed by a dynamic system equilibration under NVT ensemble is applied for pre-determined dynamic time. Dynamic time for simulated atomic structures is proportional to the number of atoms included in each supercell. A dynamic step of 0.1 fs, and a 100 kcal/mol energy deviation are kept constant for all graphene conducted simulations.

Simulations of Polymeric Matrices (Vinylester, Brominated Vinylester)

An Amorphous cell molecular dynamics module is recommended for amorphous polymers to optimize their mechanical behavior, surface characteristics, and interface interactions. An Amorphous module is a suite of computational tools that allow assembly of representative models of complex amorphous system that anticipate the key properties. Simulation parameters which are required to setup the simulation include: system composition chemical chain, temperature, and density. Representative volume element (RVE) models are established from equilibrated vinylester/brominated vinylester atomic

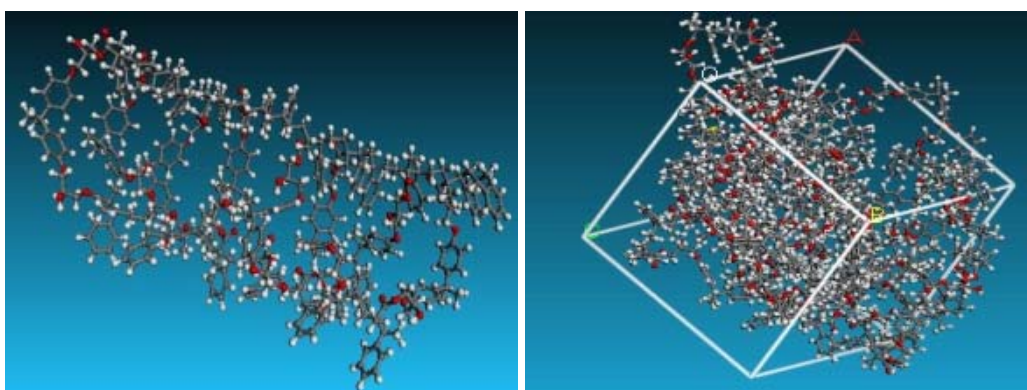
structures governed by COMPASS forcefield. The RVE is constructed of ten atomic vinyl ester/brominated vinyl ester chains each of 230 atoms. Vinyl ester simulation parameters are bulk periodic cell density 1.04 gm/cm^3 at room temperature 298K, and $T_g = 400 \text{ K}$, figure 6. Brominated vinyl ester simulation parameters are bulk periodic cell density 1.53 gm/cm^3 at room temperature 298K, and $T_g = 400 \text{ K}$, figure 7. RVE molecular systems are condensed with NPT (constant number of atoms, pressure, and temperature, MD simulations at 300K and 1 atm for 50 ps. This process is followed by NVT (constant number of atoms, volume, and temperature for 100 ps raising the molecular system temperature from 300K to 400K in stepwise dynamic simulation. For each polymeric system temperature, this is followed by an NPT dynamic step-wise temperature reduction back to room temperature 300K. Static mechanical properties are calculated for each equilibrated cell.



(a)

(b)

Figure 6. (a) Atomic vinyl ester Single Vinyl ester Chain (230) Atoms
(b) 10 Chain Vinyl ester Unit Cell (2300) Atoms



(a)

(b)

Figure 7. (a) Atomic vinyl ester Single Brominated Vinyl ester Chain (230) Atoms
(b) 10 Chain Brominated Vinyl ester Unit Cell (2300) Atoms

Simulations of Graphene Vinylester and Graphene Brominated Vinylester Interfacial Properties

The pullout energy, $E_{\text{pull-out}}$, 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, τ_i , by the following:

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

$$\tau_i = \frac{E_{\text{pull-out}}}{(W+t)L^2} \quad (2)$$

where, W , L and t are the width, length, and thickness of the graphene plate, respectively, and x is the displacement of the graphene sheet. Molecular dynamics simulations are carried out for the following fiber –polymer pull-out energies: 1. graphite –vinylester interface Figure (8), 2. graphene –vinylester interface Figure (9), 3. graphite –brominated vinylester interface Figure (10), and 4. graphene–brominated vinylester interface Figure (11).

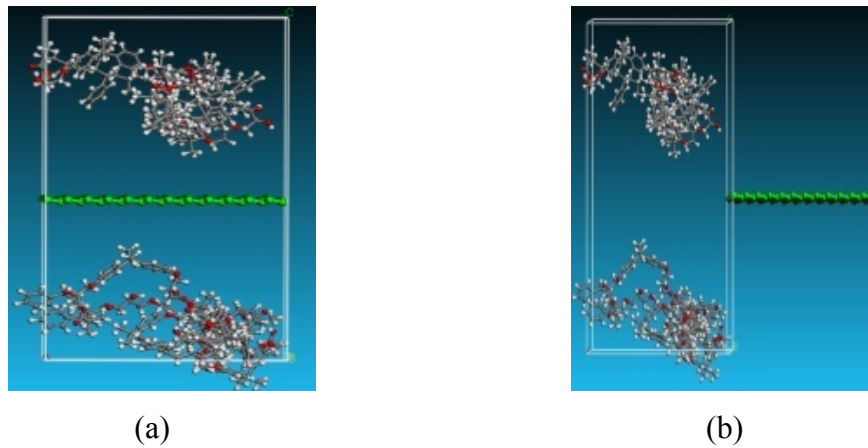


Figure 10. Atomic Model for Graphene Reinforcement Interfacial Pull-out

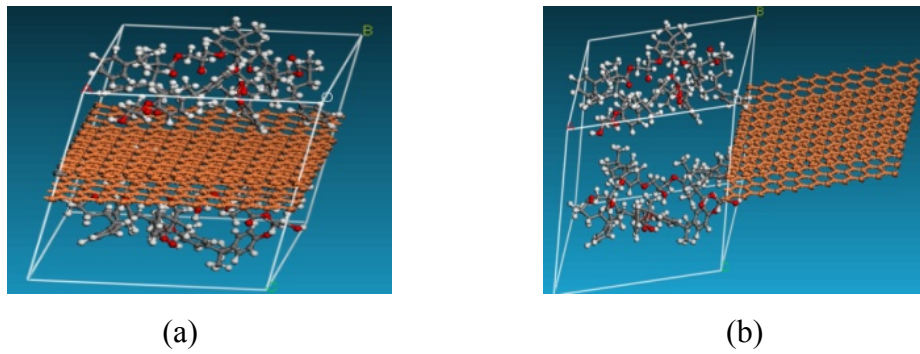


Figure 11. Atomic Model for Graphite Reinforcement Interfacial Pull-out

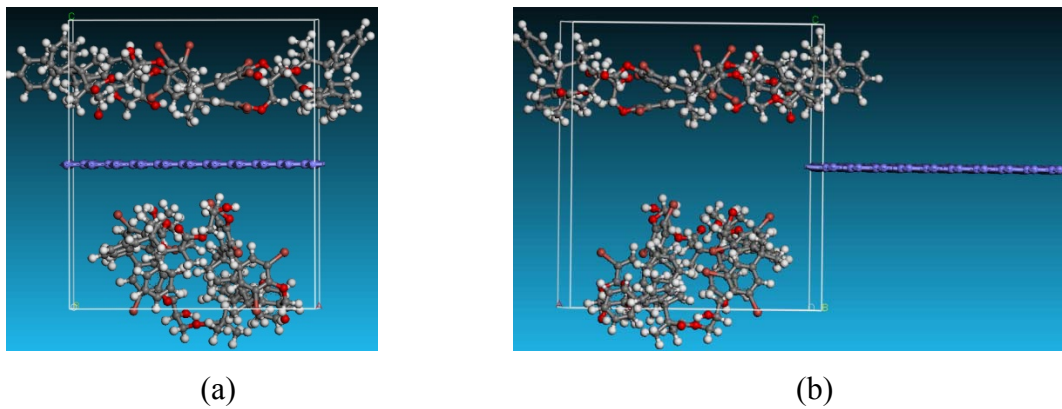


Figure 12. Atomic Model for Graphene Brominated Vinyl ester Reinforcement Interfacial Pull-out

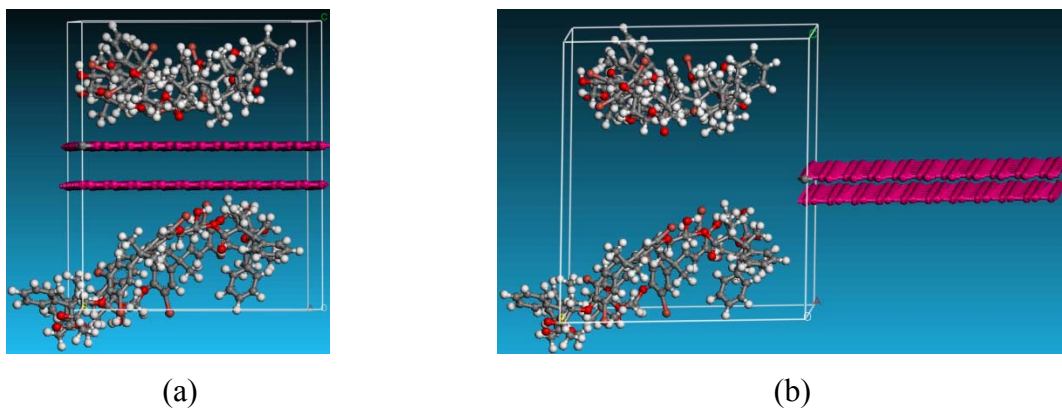


Figure 13. Atomic Model for Graphite Brominated Vinyl ester Reinforcement Interfacial Pull-out

Simulations of Graphene Composites

Simulations are carried out for 10 and 20 percent of graphite – vinyl ester figure 12(a, b), and for exfoliated graphene –vinylester composites figure 13(a, b). The simulation

conditions and cell sizes that have been constructed are mentioned later in Table VI. The NVT and NPT step simulations described earlier in matrix molecular modeling are applied to the composite simulations. Hence, the temperature of the system is maintained at 298K throughout the simulation.

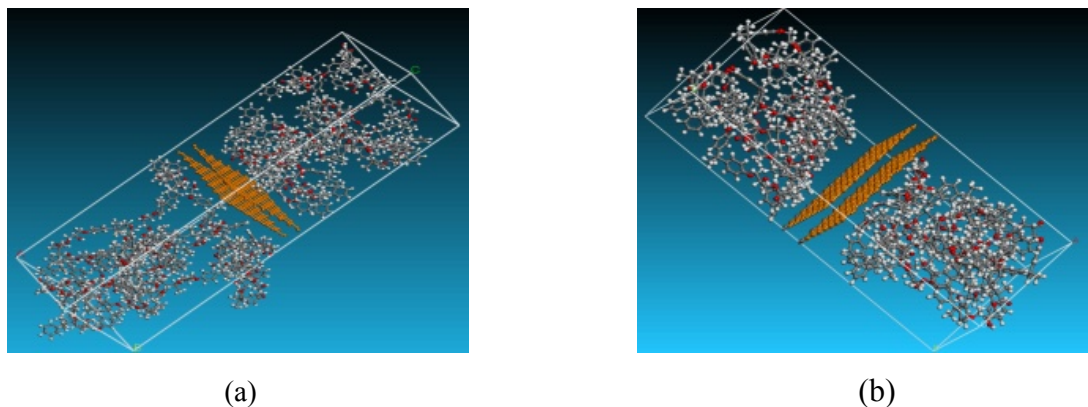


Figure 12. a) 10% Graphene Vinylester Composite, (b) 20% Graphene Vinylester Composite.

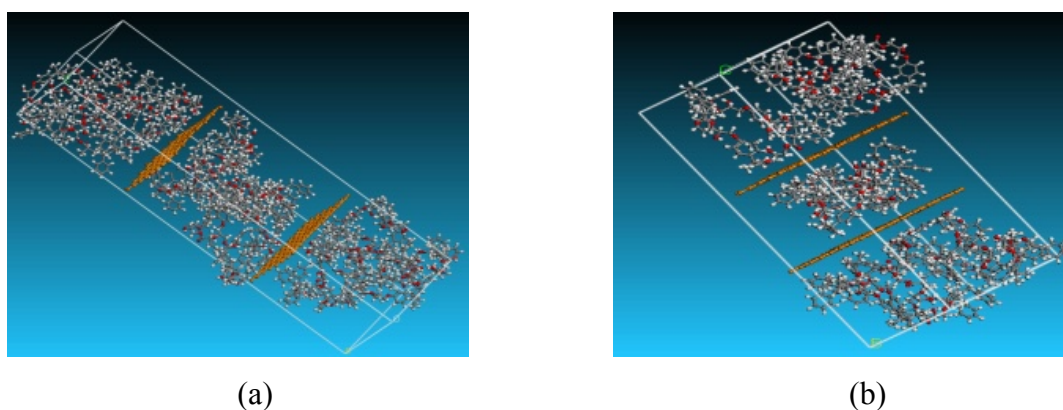


Figure 13. (a) 10% Exfoliated Graphene Vinylester Composite, (b) 20% Exfoliated Graphene Vinylester Composite.

RESULTS

Mechanical Properties of Graphene

Graphene supercells of different sizes are shown in Figure 14. Elastic constants of the numerous super cells are shown in Table I. The periodic cell size for the graphene is a 2×2 supercell crystal.

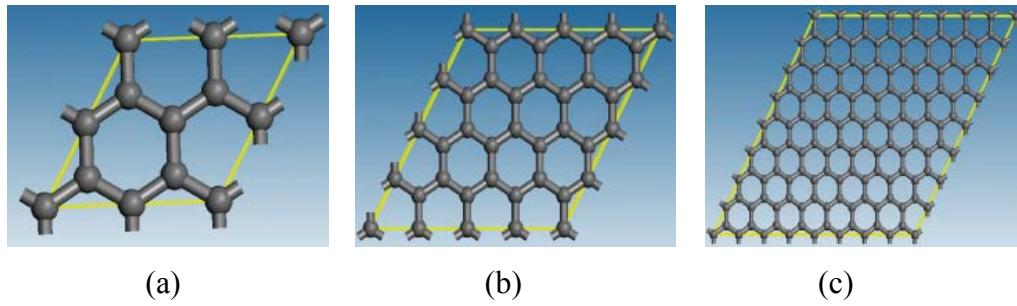


Figure 14. Graphene Atomic Supercell (a) Graphene Two Supercells, (b) Graphene Four Supercells, (c) Graphene Eight Supercells

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
ν_{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

Mechanical Properties of Graphite

Effect of Unit Cell Size

Figure 15 shows a double layered graphite molecular supercell, side and top views. Several graphite supercells are simulated to study the effect of the supercell size on graphite mechanical properties and to obtain the periodic cell dimensions for the graphite atomic structure.

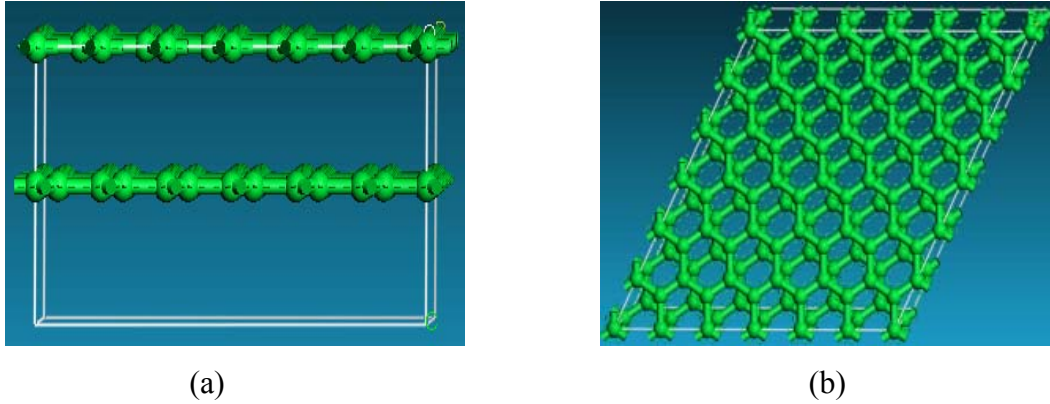


Figure 14. Double Layered Graphite Super Cell (a) Side view, (b) Top view

Table II, and Table III show the engineering constants for the graphite molecular structure of different supercell sizes. From these tables II, and III it can be seen that the engineering constants tend to remain steady for both supercell structures at 2*2 size for the double layer, and at 8*8 for the four layered graphite. Increasing the number of layers simulated requires a larger supercell to represent the periodic simulated graphite 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
ν_{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
ν_{12}	0.0	0.0
M_{23} (GPa)	406.6	406.4
K_{23} (GPa)	1015.4	1014.7

Effect of Number of Layers:

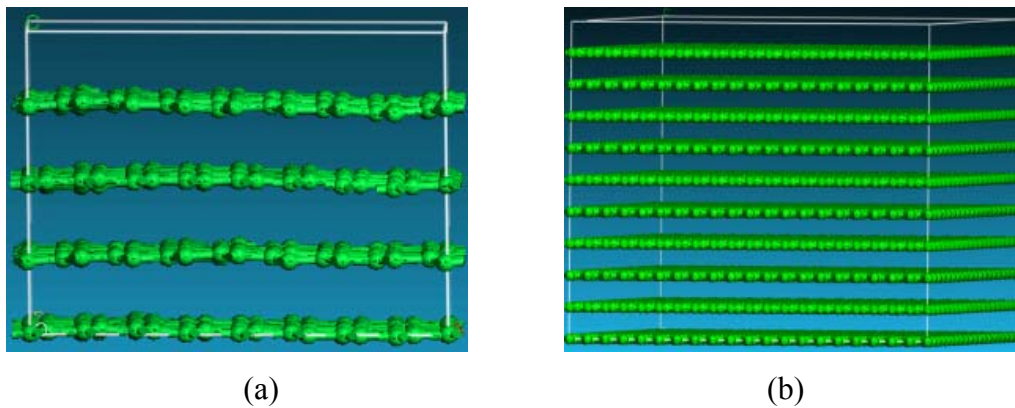


Figure 16. Multi Layered Graphite Super Cell: (a) Four Layer, (b) Ten Layer

Several layers are simulated to study their geometrical effect on graphite mechanical properties. Figure 16 shows a molecular crystal structure for a four-layered and a ten-layered graphite supercell. Table IV demonstrates the engineering constants for double, four, and ten layered graphite periodic cells. The results recorded in Table IV, affirm that the variation of the engineering constants for the multi layered graphite periodic cells is 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 (64 atoms)	4 Layers (512 atoms)	10 Layers (9640 atoms)
E_{11} (GPa)	26.9	29.2	27.8
E_{22} (GPa)	1159.6	1161.3	1160.1
ν_{12}	0.0	0.0	0.0
M_{23} (GPa)	406	406.6	406.05
K_{23} (GPa)	1014	1015.4	1015

Mechanical Properties of Vinylester

Table V shows the engineering constants of a vinylester amorphous cell for 6, 10, and 12 chains. From results shown, an amorphous cell of 10 chains of vinylester and 3200 total atoms is the periodic cell of such a polymeric structure. Hence, increasing the amorphous cell atomic size and simulated number of atoms will not induce any mechanical property variation or improvement beyond the 2300 atom periodic cell.

TABLE V. Vinylester Engineering Constants Versus Number Of Chains

Eng. Constants	6 Chains	10 Chains	12 Chains
E_{11} (GPa)	2.83	3.7	3.7
ν_{12} (GPa)	0.30	0.31	0.31

Mechanical Properties of Brominated Vinylester

Table IV demonstrates the engineering constants for a vinylester amorphous cell, of 10 chains. The results indicate as expected that the bromination of vinylester did not vastly affect the mechanical properties.

TABLE VI. Vinylester Engineering Constants Versus Number Of Chains

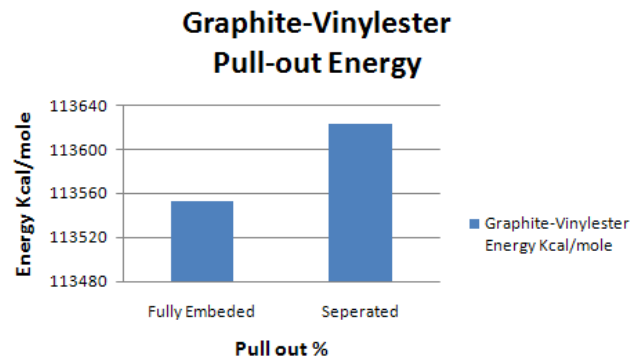
Eng. Constants	10 Chains
E11 (GPa)	3.5
ν_{12} (GPa)	0.32

Interfacial Strength

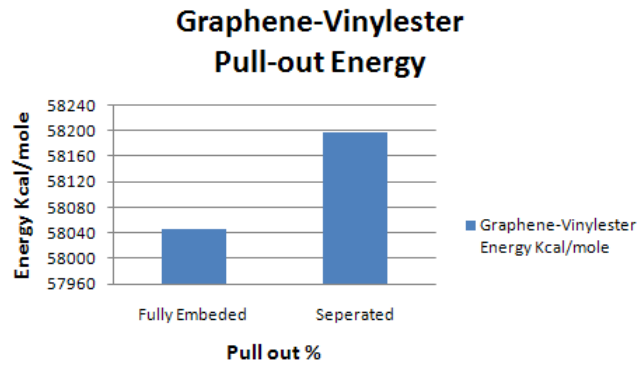
The $E_{\text{pull-out}}$ for the vinylester graphene 149.61 kcal/mol. energy plot is shown in Figure 17(a). The properties of the unit cell simulated for the pull-out energy are: density of 0.37 gm/cm^3 , molecular weight of 10672 gm/mol, and cell dimensions of (L=29.64A, W=29.64A, t=3.4A) Figure 10. According to equation 2, $\tau_i = 256 \text{ MPa}$, which is double the interfacial strength of the SWCNT- Polyethylene reported in [17, 22].

A similar atomic cell structure is constructed for the graphite (Figure 11) to study the interfacial strength of a multi layered graphene nanoplatelet. Double layered graphite is chosen with a density of 0.572 gm/cm^3 , molecular weight of 13104 gm/mol, and cell dimensions of (L=29.64A, W=29.64A, t=3.4A). $E_{\text{pull-out}}$ for the double layer of graphite is 69.8k-cal/mole Figure 17(b). The interfacial strength calculated from equation 1-2 is 125 MPa, which is less than half of the graphene interfacial strength.

Vinylester bromination effect on interfacial strength of vinylester bromination-graphene/graphite is simulated in this study. Although the mechanical properties of the brominated vinylester are comparably close to vinylester, a great interfacial strength enhancement is shown in the simulated pull-out energy configurations. Interfacial strengths summary are shown in Table V.

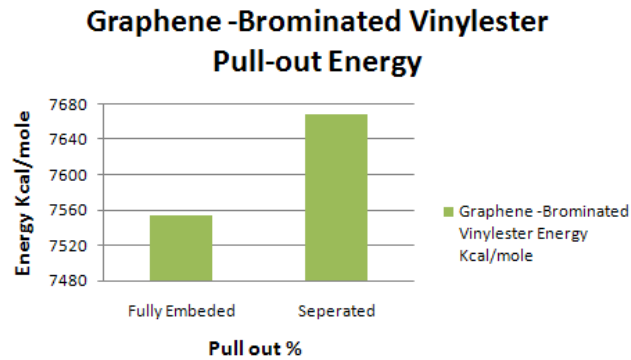


(a)

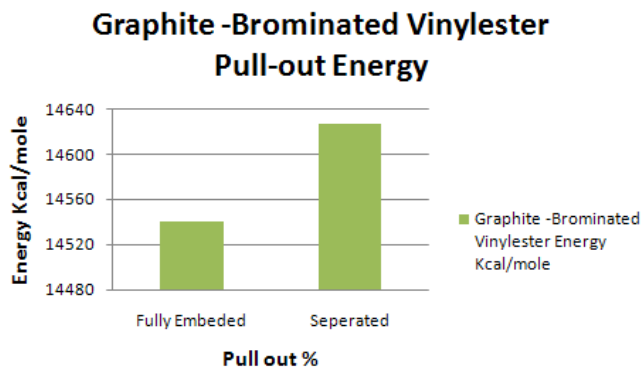


(b)

Figure 17. Potential Energy Variation for a Pull-out Test from Vinylester Matrix Composite: (a) Graphene, (b) Graphite



(a)



(b)

Figure 18. Potential Energy Variation for a Pull-out Test from Brominated Vinylester Matrix Composite: (a) Graphene, (b) Graphite

TABLE VI. Interfacial Strength for Vinylester Nanocomposites

Composite	Interfacial Strength (MPa)
SWCNT - Polyethylene	133
Graphene - Vinylester	256
Graphite -Vinylester	125
Graphene - Brominated vinylester	534.4
Graphite - Brominated vinylester	368

Molecular Dynamic Simulations of Vinylester Nanocomposites

Stiffness matrices for 10 and 20 weight percentage reinforcements are shown in Table VI. Results shown in table VI demonstrate that exfoliated graphene platelets nanocomposites have higher elastic properties than the graphite nanocomposites.

TABLE VII. Stiffness Matrices of GNP- Vinylester Nanocomposite

GnP -Vinylester Composite Stiffness Matrix: 10%	
Unit Cell size: (19.76*19.76*58.6) A	
Triclinic cell: $\alpha=\beta=90^\circ$, $\gamma=120^\circ$	
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: $\alpha=\beta=90^\circ$, $\gamma=120^\circ$

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: $\alpha=\beta=90^\circ$, $\gamma=120^\circ$

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: $\alpha=\beta=90^\circ$, $\gamma=120^\circ$

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

- From Table I Graphene had an E_{11} of 1.3 TPa, in plane graphite sheet direction
- Number of layers has minimal effect on simulated mechanical engineering for multi layered graphite periodic cells
- The periodic unit cell size of vinyl ester atomic structure consists of 2300 atoms, and mechanical engineering properties of $E=3.7$ GPa and $\nu = 0.31$
- Interfacial strength for the graphene came out to be double the interfacial strength of the double layered of graphite
- Graphite and CNT have comparable interfacial strengths
- Bromination of vinyl ester has highly enhanced the interfacial strength.

ACKNOWLEDGEMENT

This work was partially supported by the funding received under a subcontract from the Department of Homeland Security-Sponsored Southeast Region Research Initiative (SERRI) at the Department of Energy's Oak Ridge National Laboratory, USA.

REFERENCES

1. Lan, T. T.; Kaviratna, P. D.; Pinnavaia, T. J. *Journal of Chemistry of Materials*, **1995**, 7(11), 2144.
2. Lan, T. T., Pinnavaia, T. J. *Mat. Res. Soc. Symp. Proc.* **1996**, 435.
3. Vaia, R. A., Price, G., Ruth, P. N., Nguyen, H. T., Lichtenhan, J. *Applied Clay Science*, **1999**, 15(1), 67.
4. LeBaron, P. C., Wang, Z., Pinnavaia, T. J. *Applied Clay Science*, **1999**, 15(1), 11.
5. Varley, R., J., Groth, A., M., Leong, K., H. *Composite Science and Technology*, **2007**, 68, 2882.

6. Meyer, J. C., Geim, A. K., Kastnelson, M. I., Novoselov, K. S., Booth, T. J., Roth, S. *Nature*, **2007**,446,60.
7. Figiel, L., Buckley, C. P. *Computational Materials science*, **2008**, in press.
8. Valavala, P.K., Odegard, G.M. *IUTAM Symposium on Modelling Nanomaterials and Nanosystems:Proceedings of the IUTAM Symposium, Aalborg, Denmark, 2008*,19.
9. Zeng, Q. H., Yu, A. B., Lu, G. Q. *Progress in Polymer Science*, **2007**, 33,191.
10. Harkin- Jones, Figiel, Spencer, Abu-Zurayk, Al-Shabib, Chan, Rajeev, Soon, Buckley, at. el. *Plastics, Rubber & Composites*, **2008**, 37(2), 113.
11. S. Mouras, et al. *Revue de Chimie Minerale*, **1987**, 24:572.
12. Novoselov, A. K., Geim, A. K., Morsozov, S. V., Jaing, D., Zhang, Y., Dubonus, S. V., Grigrieva, I.V., Firsov, A. A. *Science*, **2004**,Oct 22.
13. Novoselov, K. S., Jaing, D., Booth, T. J., Khotkevich, V. V., Morzov, S. V., Geim, A. K. 2005. *PNAS*, 102(30), 10451.
14. Lee, C., Wei, X., Kysar, J. W., Hone, J. *Science*, **2008**, 321,385.
15. Wikipedia
16. Karger-Kocsis, J., Gryshchuk, O., Schmitt, S. *Journal of Materials Science*, **2003**, 38(3),413.
17. Derkane Momentum™ 640-900. Epoxy Vinyl Ester Resin, **2004**.
18. Gou, J., Minaie, B., Wang, B., Liang, Z., Zhang, C. *Computational Materials Science*, **2004**, 31,225.
19. Wagner, H. D., Vaia, R. A. *Materials Today*, **2004**, 38.
20. Liao K, Li, S. *Applied Physics Letters*, **2001**, 79 (25), 4225.
21. Xiao, M., Sun, L., Liu, J., Li., Y., Gong, K. *Polymer*, **2001**, 43,2245.
22. Leach, R. A. "Molecular Modeling Principles and Application," Pearson Education, EMA. **2001**.
23. Al-Ostaz A., Pal, G. *Journal of Materials Science*, **2008**, 43,164.
24. MS Modeling 4.0 Online Help Manual, Accelrys Inc., **2005**
25. Sun, H. *Journal of Physical Chemistry B*, **1998**, 102, 7338.