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Mechanical Behaviour of Graphene Reinforced Aluminum Nano composites

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Abstract

In this paper, molecular dynamics (MD) simulations are performed on graphene-aluminum (GS-Al) nanocomposite. The mechanical properties of the nanocomposite are investigated by the application of uni-axial load on one end of the representative volume element (RVE) and fixing the other end. The interactions between the atoms of Al are modelled using Embedded Atom Method (EAM) potentials, whereas Adaptive Intermolecular Reactive Empirical Bond-Order (AIREBO) potential is used for the interactions among carbon atoms and these pair potentials are coupled with the Lennard-Jones (LJ) potential. The result shows that the incorporation of Gn into the Al matrix can increase the Young's modulus of the nanocomposite substantially. The nanocomposite containing 6.7 vol.%of GS exhibits Young's modulus of 143.8 GPa and 116.8 GPa along longitudinal and transverse directions, respectively that are 82.8% and 46.5% higher than pure Al. Results from the molecular dynamics simulations are also compared with analytical results obtained from semi-empirical Halphin-Tsai (H-T) model and the Rule of Mixtures (ROM).

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*Keywords:*Molecular dynamics (MD); graphene; nanocomposites; mechanical properties; representative volume element (RVE)

1. Introduction

Graphene, an one-atom thick, two-dimensional sheet of carbon atoms is attracting the attention of researchers around the world due to its excellent mechanical, electrical and thermal properties [1, 2]. With such properties, graphene sheets (GSs) are considered as ideal material for composite reinforcement in polymer, metals and ceramics. Many studies are available in literature related to investigation of the mechanical properties of graphene reinforced polymers [3-6], but there are scarcity of studies on GS reinforced metal nanocomposite. This is likely a result of the greater difficulties in the dispersion and fabrication, and the unknown interfacial chemical reactions in metal

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composites. Among the metal matrices, Aluminum (Al) is mostly used matrix material due to its diverse range of technical applications for lightweight alloys. Recently, Wang et.al [7] fabricated Al composites reinforced with GS based on flake powder metallurgy, and reported that, by adding only 0.3 wt.% of GS in Al matrix the ultimate strength of resulting composite enhances by 62%.

There are enormous challenges in the experimental development and characterizations of GS-based nanocomposites because of difficult and expensive processes involved. At the same analytical models at nanoscale are either difficult to establish or too complicated to solve. Therefore, cost-effective and less time-consuming computational approaches play a significant role in the development and characterization of GS based nanocomposites to provide simulation results for better understanding, analysis and design of such nanocomposites. Molecular Dynamics (MD) is frequently used by the researchers [8-11] around the world to study the polymer and metal nanocomposites owing to its specific capabilities to capture the effect of force field between the atoms. Rahman& Foster [12] investigated through MD the deformation mechanism of GS in a graphene reinforced polyethylene (PE) nanocomposite and reported that GS enhances the overall Young's modulus and tensile strength of GS-PE nanocomposite by 60% and 54.1%, respectively, for the weight fraction of 5%. The effect of GS orientation on the Young's modulus and strength was also studied by Rahman& Foster [12]. Hadden et al.[4] studied the effect of volume fraction of graphenenanoplatelets (GNPs) on the mechanical strength of GNP/carbon fiber/epoxy hybrid composites, and observed a substantial effect of GNP volume fraction and dispersion on the transverse mechanical properties of the hybrid composite while the axial properties are found to be less influenced.Zhang & Jiang [13] explained using MD the structural and mechanical properties of the GS/graphene oxide paper based polymer composites.

The aim of the present paper is to investigate the mechanical properties of GS reinforced Al nanocomposite under uni-axial loading using molecular dynamics.To validate the procedure, Young's modulus of GS is predicted using MD and the obtained values are compared with the available results in literature. In addition, the results of current study are compared with that obtained by semi-empirical Halphin-Tsai (H-T) model and the Rule of Mixture (ROM).

2. Molecular Dynamics simulation

Molecular Dynamics simulations have been performed on Al/GS nanocomposite using open source simulation engine, Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)[12] distributed by Sandia national laboratories. Another source code VMD (Visual Molecular Dynamics)is utilized to model the graphene sheet and to visualize the results obtained from the LAMMPS simulation. The GS of area 25 nm^2 having 1008 carbon atoms is embedded into the Al matrix such that armchair configuration lies along *y*-direction in the representative volume element (RVE), whereas the Al matrix has the shape of cube with side of $50A^0$, as shown in Fig. 1. In order to place the GS inside the Al matrix and to avoid premature rupture of Al–Al and C–C bonds, an equilibrium distance between C and Al atoms is taken as, $h = 0.8485\sigma$ [8], where σ is the van der Waals radius parameter of Lennard-Jonnes (LJ) potential for the non-bonded interphase zone between GS and Al matrix.

The Al matrix has 7500 atoms and Embedded-Atom Method (EAM) potential is used to model the atomic forces among Al atoms. The total energy E_i of an atom *i*is given by [14],

$$E_i = F_\alpha\left(\sum_{j\neq i}\rho\beta\left(r_{ij}\right)\right) + \frac{1}{2}\sum_{j\neq i}\emptyset_{\alpha\beta}\left(r_{ij}\right) \quad (1)$$

Where F is the embedding energy which is a function of the atomic electron density ρ, Øis a pair potential interaction, and α, β are the element types of atoms *i* and *j*. The multi-body nature of the EAM potential is a result of the embedding energy term. Both summations in the formula are over all neighbours *j* of atom *i* within the cut-offdistance.

Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential is used to simulate the inter-atomic forces between the carbon atoms, which is given in following form,

$$E = \sum_i\sum_{j\neq 1}\left(E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k\neq i,j}\sum_{l\neq i,j,k}E_{kijl}^{TORSION}\right) \quad (2)$$

Where E^{REBO} corresponds to the short range interactions between covalently bonded pair of atoms, E^{LJ} is the Lennard-Jones (LJ) potential used for long range interactions i.e. non-bonded pairs of atoms and $E^{TORSION}$ (torsional potential) depends on the neighbouring atom's dihedral angles.

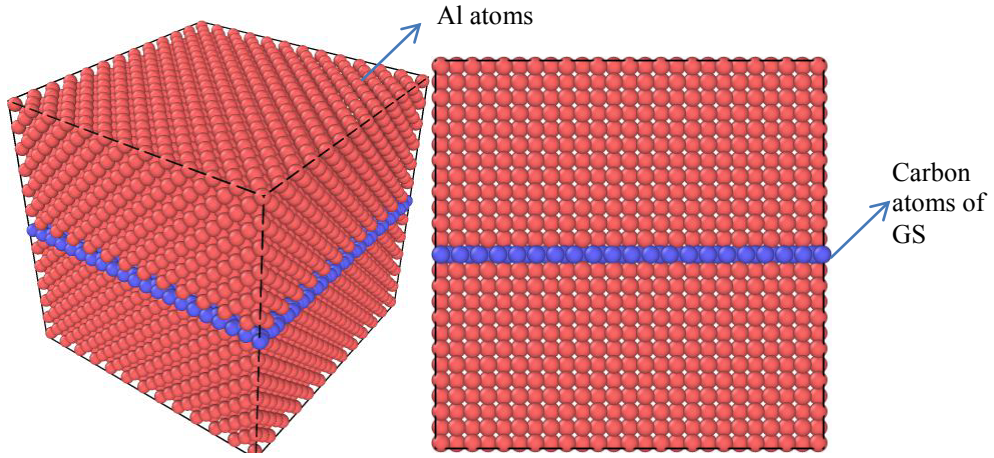

Fig.1. RVE containing single layer GS in Al matrix

The long range LJ 12-6 potential is further deployed to account for the non-bonded interactions between carbon atoms of graphene and atoms of Al matrix.

$$E = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], r < r_c \qquad (3)$$

Where, r_c is the *LJ* cut-off radius beyond which van der Waals interaction is negligible and it is taken equal to 2.5 σ. The parameters ε and σ are the coefficients of depth of potential well and equilibrium distance, respectively. These parameters for the interactions between carbon atoms and Al atoms are computed using widely used Lorentz Bertholet (LB) rule [8] and given as σ = 3.1325 A and ε = 0.003457 eV. The values of LJ potential parameters for Al and C atoms are listed in Table 1.

Table 1: L-J pair potential parameters for C and Al atoms

L-J Potential parameters	Carbon, C	Aluminum, Al
$\sigma(A^0)$	3.41500	2.8500
ε[eV]	0.00239	0.0050

In order to stabilize GS/Al nanocomposites, an initial equilibration analysis for 20000 time steps is performed with each timestep equal 1 fs. To avoid internal residual stresses of RVE the total energy was reduced to minimum value. Fig. 2 shows the variation of total energy (eV) with respect to relaxation steps and it is found that the system reaches the equilibrium position after 20ps. The simulation was performed at room temperature,taken as 300 K. The equilibrated molecular structure was accomplished by performing the sequence of NVT and NPT ensembles, where NVT ensemble stands for constant volume (V) and temperature (T) conditions of fixed number of atoms (N) during the simulation, and NPT constant pressure (P) and temperature (T) conditions of fixed number of atoms (N) during the simulation. After the equilibration process, MD simulation is carried under NVT conditions by fixing the one end of the RVE and by giving a constant velocity of 0.1 A^0/ps to the other end. MD simulation runs for 10000 time steps with each time step equal to 1 fs.

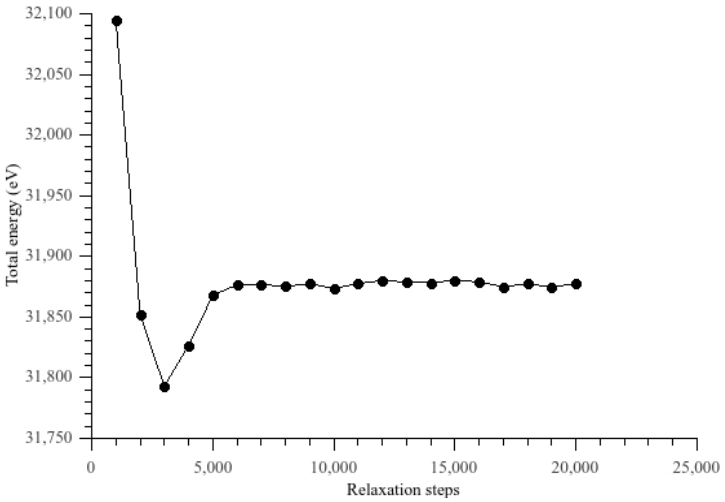

Fig.2. Total energy variation in the equilibration process

3. Validation

In order to verify the procedure followed in the current work to study the stress-strain behaviour of GS reinforced Al nanocomposite, mechanical properties of GS of dimensions $50A^0 \times 50A^0$are predicted and compared with the available results in the literature.The x- and y-directions as marked in Fig. 3 are taken astransverse and longitudinal, respectively.Initially, GS is divided into three groups of atoms called upper, lower and middle. A velocity of $0.3A^0$/ps is given to the upper group of atoms while fixing the lower group of atoms (refer Fig. 3). The stress-strain curves of a GS along longitudinal and the transverse directions obtained from the simulation are shown in Fig.4. The obtained values of Young's modulii of the GS in the longitudinal and the transverse directions are 952.6GPa and 883.5 GPa, respectively, and these values are in good agreement with the results in the literature [15].

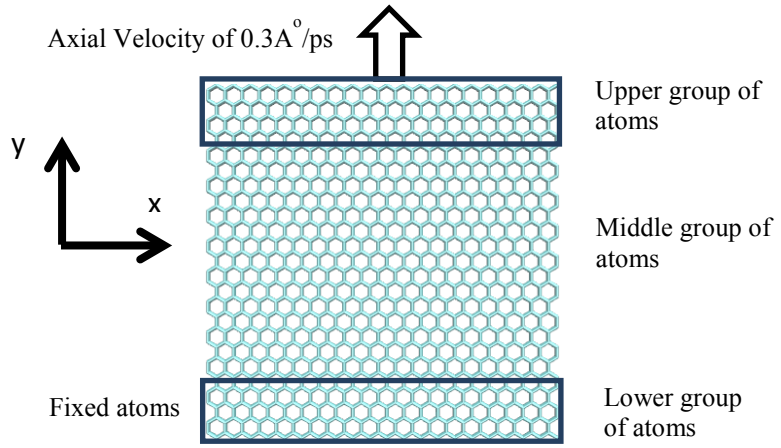

Fig.3. Schematic illustration of the tension test on GS along the longitudinal direction

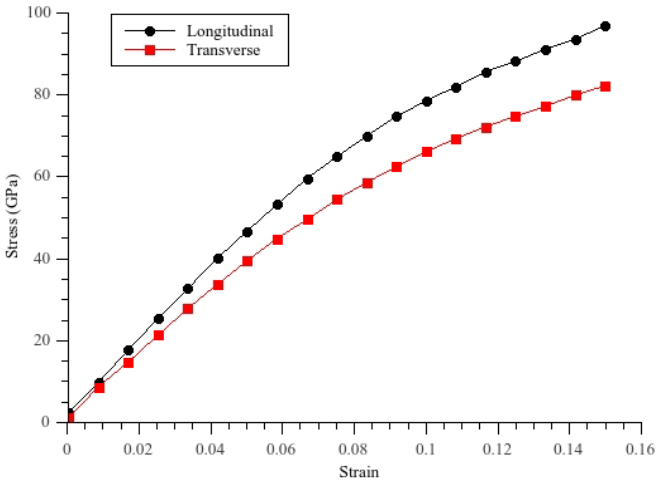

Fig.4. Stress-Strain curves of GS along the longitudinal and the transverse direction

4. Results and Discussion

The selected representative volume element (RVE) as shown in Fig.1 is subjected to similar equilibration and loading process to study the stress-strain behaviour of the GS-Al nanocomposite under tensile loading. Obtained comparative results between the tensile behaviour of GS and GS-Al nanocomposite in longitudinal and transverse directions are plotted in Fig. 5. For the volume fraction of 6.7%, the Young's modulus of the nanocomposite is found to be 143.8GPa along the longitudinal (E_l) direction and 116.8 GPa along the transverse (E_t) direction which are,respectively, 82.8% and 48.6% more than that of pure Al.

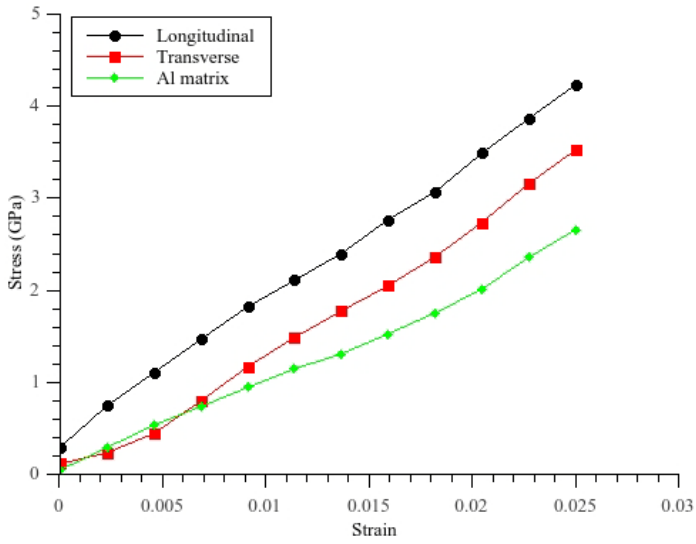

Fig.5. Stress-Strain curves of Al and GS-Al nanocomposite along longitudinal and transverse direction

The semi-empirical Halpin-Tsai (H-T) model and the Rule of Mixtures (ROM) [6] arealso used in the present work to compare the modulus of GS-Al nanocomposite. From the H-T model, which is used to predict the Young's modulus of uni-directional or randomly distributed filler-reinforced nanocomposites, the Young's modulus of nanocomposite (E_C) for uni-directional GS in Al matrix is given by

$$E_c = E_m\left(\frac{1+\eta_L \xi V_c}{1-\eta_L V_c}\right) \quad (4)$$

$$\eta_L = \frac{\left(\frac{E_g}{E_m}\right)-1}{\left(\frac{E_g}{E_m}\right)+\xi} \quad (5)$$

$$\xi = 2\alpha_g /3 = 2l_g/3t_g \quad (6)$$

Where E_c represents Young's modulus of the nanocomposite in which GS aligned parallel to the matrix surface. E_g and E_m are the moduli of GS and matrix, respectively. α_g, l_g andt_g represent aspect ratio, length and thickness of GS, and V_c is the volume fraction of GS in the Al matrix.For longitudinal direction E_g and $E_m$are 952.61 and 78.64 GPa respectively. The thickness of GS is considered as $3.4A^0$, and length of GS is $50A^0$. While in the transverse direction $E_g$of the GS is 883.45 GPa and remaining values are same as the longitudinal direction. Elastic modulus obtained from MD and H-T methods are listed in table 2.

For a composite under uni-axial loading the elastic modulus can be predicted by conventional macroscopicROM as well. It is given by

$$E_c = V_c E_g + (1 - V_c)E_m \quad (7)$$

Where E_c, Eg and E_m are the modulus of nanocomposite, GS and matrix, respectively; V_c is the volume fraction of GS in the Al matrix. Results obtained from the ROM are also shown in Table 2.The difference in the obtained results is due to the fact that in contrast to MD simulation study, the bonding between matrix and reinforced materials is assumed to be perfect in micromechanics models (i.e., H-T and ROM) and these models are largely depend on reinforcement geometry, packing geometry and loading condition.

Table2**:** Elastic moduli (in GPa) of GS reinforced Al composite ($V_f = 0.067$)

Elastic constants	MD	H-T	ROM
E_l	143.8	108.5	137.2
E_t	116.8	107.2	132.6

5. Conclusion

Mechanical properties of GS-Al nanocomposite are predicted in the present study using molecular dynamics simulation. Stress-strain behaviour of the nanocomposite is obtained by the application of constant velocity at the one end of RVE keeping the other end fixed. The linear region of stress-strain curve is utilized to estimate the Young's modulus of the nanocomposite. From the simulation results, it is established that, in comparison with pure Al, The Young's modulus of nanocomposite increased by 82.8% in the longitudinal direction and 46.5% in the transverse direction for the volume fraction of 6.7%. Thus, embedding of GS into Al matrix improves the stiffness property substantially. The results obtained from the MD simulation are also compared with the theoretical results obtained using H-T and ROM models.

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