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Graphene Engendered aluminium crystal growth and mechanical properties of its composite: An atomistic investigation

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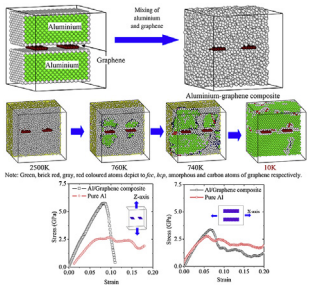
HIGHLIGHTS

- Aluminium atoms aggregate over the graphene to minimize the energy of the system.
- Graphene facilitates the crystallization of aluminium during the solidification process.
- Aluminium atoms organized in *fcc* {111} structure interface.
- Excellent strenght found during deformation along normal to the graphene.

GRAPHICAL ABSTRACT



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ABSTRACT

Aluminium/graphene nanocomposite shows a combination of many useful properties, such as light weight, good mechanical, extremely high electrical and thermal properties. Crystal growth of aluminium at the aluminium/graphene interface highly influences the above mentioned properties. In this paper, the orientation of aluminium atoms along with mechanical properties of aluminium/graphene nanocomposite have been studied by using molecular dynamics simulation. The aluminium atoms were organized in face-centred cubic lattices in bulk. However, at the aluminium/graphene interface, aluminium atoms were organized in the {111} facet of the face-centred cubic. The aluminium/graphene nanocomposite shows significantly improved mechanical properties compared to pure aluminium. The Steinhardt-Nelson order parameters, adaptive common neighbor analysis, radial distribution function, and potential energy evolution have been used to characterize the orientation of aluminium in presence of graphene sheets. The main outcomes of this study may provide a detailed understanding of the interfacial properties of graphene–aluminium nanocomposites systems, which help to enhance the performance of graphene-based nanocomposites materials.

1. Introduction

The aluminium/graphene nanocomposite shows improved properties compared to pure aluminium such as high mechanical strength [1–3], good electrochemical properties can be considered as an anode material for battery [4], highly conductivity and transparent nature leads to use in making next generation solar cell [5]. An understanding of the orientation of aluminium atoms near a graphene substrate is vital in the development of high-performance aluminium/graphene nanocomposites systems. Most of the research groups have been reported that the responsible factors for enhancing the properties of aluminium graphene nanocomposites are dispersed/aggregation, concentration of

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nanofillers and processing methodology [6–14]. However, Li et al. [6] have studied the microstructural and tensile properties of aluminium/graphene nanoflake composite and it relates to the properties of the interface between aluminium and graphene by using experimental technique. They have observed a significant enhancement in mechanical strength over to pure aluminium. Also, they have assumed that each aluminium grain adsorb evenly on the graphene substrate. But some issues still remain open yet, such as orientation of aluminium atoms over the hexagonal structure of graphene substrate and interface characteristics. In this paper, i have resolved these issues by using molecular dynamics simulation. Molecular dynamics simulation provides us some precise advantages over other experimental techniques such as, easy to forecast the properties of materials, at very high or low pressure situation which is difficult through experiments.

The molecular dynamics simulation technique has been used by a few researchers to study the various properties of aluminium nanocomposites [15–20]. Mainly, they have studied the compressive/tensile strength, stability of nanocomposite material at high temperature, buckling behavior of carbon nanotubes etc. Silvestre et al. [16] have studied the properties of Aluminium/Carbon nanotubes composite by using molecular dynamics simulations. They have found that the Aluminium/Carbon nanotubes composite illustrate improved mechanical properties, etc. However, they have not discussed the orientation of aluminium atoms on the carbon nanotube substrate. Choi et al. [17] have studied the effect of carbon nanotubes inclusion in aluminium on the mechanical properties by using molecular dynamics simulation. They have found that the Young's modulus and toughness of aluminium/carbon nanotubes increases significantly. Despite of these studies, the orientation of aluminium atoms over the graphene sheet and its mechanical propertieas still needs to be explored by molecular dynamics simulation. To the best of my knowledge, the orientation/crystallization and mechanical properties of aluminium/graphene nanocomposites by using MD simulation have not been studied earlier in the light of published literature.

In this study, I have studied the orientation of aluminium atoms over the graphene substrate along with mechanical properties by using molecular dynamics simulation. The adaptive common neighbor analysis and Steinhardt-Nelson bond orientation order parameters have estimated to conduct an accurate characterization of structural orientation of aluminium atom over the graphene substrate. Variation of potential energy of aluminium as a function of decreasing temperature has been studied to elucidate the phase transition phenomena. The choice of simple monoatomic metal such as aluminium allows us for the simulation, that interact primarily through Van der Waals interaction potential with the graphene substrate. Graphene has been chosen as a substrate because of its well-defined, regular hexagonal ring structure made of carbon atoms. The behavior of aluminium atoms on graphene substrates is perhaps the simplest system that allows us to focus on the structural orientation of the atoms.

2. Simulation details

The constant temperature molecular dynamics simulation has been used to study the various properties of aluminium/graphene composite [35]. Large scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [21], Open Visualization tool (OVITO) [22] and Visual Molecular Dynamics (VMD) [23] software packages implemented to conduct molecular dynamics simulation, visualization/analysis of aluminium/graphene nanocomposite. The embedded atom method (EAM) potential with Finnis-Sinclare has been used for the interaction potentials between aluminium atoms as details given by Mendelev et al. [24]. The total interaction potentials between aluminium atoms, E_{Al} is calculated by

$$E_{Al} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \varphi_{ij}(r_{ij}) + \sum_{i=1}^{N} F_i(\rho_i) \quad (1)$$

where the subscripts i and j represents the aluminium atoms, N is the number of aluminium atoms in the simulation system, r_{ij} is the separation between two aluminium atoms i and j, φ_{ij} is the pair potential of atoms i and j, and $F_i(\rho_i)$ represents the embedding energy of atom i with electron density ρ_i.

$$\rho_i = \sum_j \psi(r_{ij}) \quad (2)$$

Where $\psi(r_{ij})$ is the electron density of aluminium atom i from a neighbouring aluminium atom j.

The interaction parameters between aluminium atom and the carbon atom of graphene have been calculated by 12-6 Lennard Jones potential as given in equation (3).

$$E_{LJ} = 4\varepsilon_{Al-C}\left[\left(\frac{\sigma_{Al-C}}{r}\right)^{12} - \left(\frac{\sigma_{Al-C}}{r}\right)^{6}\right] \quad (3)$$

Where ε_{Al-C}, and σ_{Al-C} are the Lennard Jones parameters for energy and equilibrium interatomic distance between aluminium and Carbon atom of graphene at the null point respectively. The values of ε_{Al-C} and σ_{Al-C} were determined with Lorentz-Berthelot mixing rule parameter. The value of ε_{Al-C} was obtained from the geometric average ($\varepsilon_{Al-C} = \sqrt{\varepsilon_{Al-Al} \times \varepsilon_{C-C}}$) between ε_{Al-Al} (aluminium-aluminium) and ε_{C-C} (carbon atom of graphene). The value of σ_{Al-C} was obtained from the arithmetic average ($\sigma_{Al-C} = \frac{(\sigma_{Al-Al}+\sigma_{C-C})}{2}$) between σ_{Al-Al} (aluminium) and σ_{C-C} (carbon atom of graphene). The values of Lennard Jones parameters for energy and equilibrium interatomic distance of carbon atoms of graphene $\varepsilon_{C-C} = 0.00296eV$ and $\sigma_{C-C} = 3.407\AA$, and for aluminium atoms $\varepsilon_{Al-Al} = 0.4157\ eV$ and $\sigma_{Al-Al} = 2.62\AA$ have been adopted from Refs. [25,26]. The values of Lennard Jones parameters for the C-Al interface [16] has been used $\varepsilon_{Al-C} = 0.035078eV$ and $\sigma_{Al-C} = 3.0135\AA$. The MD simulation is carried out in an NPT ensemble, in which number of atoms (N), simulation temperature (T) and pressure (P) are conserved. The Nose-Hoover thermostat [27,28] has been implemented to maintain the appropriate temperature and pressure of the system along with velocity-Verlet algorithm [29] with a time step of 1 femto-second.

2.1. Parameter studied

2.1.1. Adaptive common neighbor analysis (a-CNA)

The *a-CNA* methodology is a most frequently used for structure identification methods in metals, metal matrix-nano composite and alloys. It provides an accurate or precise organization of local atomic arrangements of atoms, such as *fcc, bcc, hcp, ico* and other. OVITO package [30] has been used to compute adaptive a-CNA for each aluminium atom in during cooling process.

2.1.2. Bond order parameters (BOP)

The bond order parameters [31–33], namely, Q_6, $\widehat{W}_6$, Q_4 and $\widehat{W}_4$ have been calculated to characterize the orientation of aluminium atoms over the graphene substrate. The bond orientational order parameters $Q_{lm}(r)$, associated with neighboring aluminium atoms are the set of numbers calculated by using the following equations