



Characterizing mechanical properties of graphite using molecular dynamics simulation

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ABSTRACT

The mechanical properties of graphite in the forms of single graphene layer and graphite flakes (containing several graphene layers) were investigated using molecular dynamics (MD) simulation. The in-plane properties, Young's modulus, Poisson's ratio, and shear modulus, were measured, respectively, by applying axial tensile stress and in-plane shear stress on the simulation box through the modified NPT ensemble. In order to validate the results, the conventional NVT ensemble with the applied uniform strain filed in the simulation box was adopted in the MD simulation. Results indicated that the modified NPT ensemble is capable of characterizing the material properties of atomistic structures with accuracy. In addition, it was found the graphene layers exhibit higher moduli than the graphite flakes; thus, it was suggested that the graphite flakes have to be expanded and exfoliated into numbers of single graphene layers in order to provide better reinforcement effect in nanocomposites.

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1. Introduction

With the characteristics of high strength and stiffness, the graphite has been used as reinforcements in composite materials [1]. The natural graphite is constructed by numbers of graphene layers with interlayer spacing of around 3.4 Å. Through chemical oxidation in the environment of sulfuric and nitric acid, the acid intercalant can be intercalated into the graphite galleries to form an intercalated graphite compound. Subsequently, by applying rapid heating because of the vaporization of the acid intercalant in the graphite galleries, the interacted graphite was significantly expanded along the thickness direction and converted into the expanded graphite (EG). After a mechanical mixer together with sonication process, the expanded graphite was dispersed and exfoliated into the polymer matrix to form graphite-reinforced nanocomposites. The synthesizing process for manufacturing the nanocomposites was discussed in detail in the literatures [2,3]. Recently, Si and Samulski [4] employed platinum nanoparticles adhered to the graphene to prevent the aggregation of isolated graphene sheets during the drying process. However, the stacked graphene structures (so called graphite flakes) are commonly observed in TEM micrographs and XRD examination [5], and it is a challenging task to fully exfoliate the aggregated graphene sheets. In fact, graphite flakes together with graphene layers are commonly observed in graphite nanocomposites and it is important to clarify if the two atomistic configurations of the graphite,

i.e., graphite flakes and single graphene layer, would have the same mechanical properties. Moreover, in order to accurately characterize the mechanical properties of the graphite-reinforced nanocomposites, an exploration of the fundamental properties of the graphite associated with different microstructures is required.

Cho et al. [6] performed a molecular structural analysis to calculate the graphite's elastic constants. The in-plane properties of graphite were derived by considering the geometric deformation of a single graphene sheet subjected to in-plane loading. However, for the out-of-plane properties, they modeled the graphic as graphic flake with multi graphene layers, the non-bonded atomistic interactions of which were described using Lennard-Jones potential function. Scarpa et al. [7] proposed truss-type analytical models in conjunction with cellular material mechanics theory to describe the in-plane elastic properties of single layer graphene sheets. It was found that the analytical results and the numerical results obtained from finite element shows good agreement with existing numerical values. Hemmasizadeh et al. [8] who correlated the force-depth results obtained from MD simulation with the large deflection formulation of circular plates loaded at center to evaluate the effective Young's modulus of graphene sheet and the corresponding wall thickness of the single sheet. By using MD simulation, Bao et al. [9] investigated the variations of Young's modulus of graphite, which contains different numbers of graphene layers (one to five layers). Results indicated that there is no considerable difference in Young's modulus between the single layer of graphene and graphite flakes with five layers of graphene. Reddy et al. [10] modeled the elastic properties of a finite-sized graphene sheet using continuum mechanics approach based on

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Brenner’s potential [11]. The computed elastic constants of the graphene sheet are found to follow the orthotropic material behaviors. In addition to the fundamental material properties, the vibrational responses of single layer graphene sheets were investigated through a molecular structural mechanics approach [12]. Both mode shapes and natural frequency of single graphene sheet were considered in their analysis. In light of the forgoing, most studies characterize the elastic properties of the graphite based on the behavior of a single graphene sheet; the mutual influences of the adjacent graphene layers on the mechanical responses in the graphite flakes are rarely taken into account. As previously mentioned, both the graphene layer and the graphite flakes were commonly found in the nanocomposites, so it is not adequate to utilize the properties of the graphene sheet instead of the graphite flakes in the modeling of graphite-reinforced nanocomposites.

In this study, the mechanical properties of the graphite flakes and the graphene were systematically characterized using MD simulation. Both bonded and non-bonded interactions were accounted for in the description of the atomistic graphite structures. By applying uniaxial tensile loading on the atomistic graphite structures, the Young’s modulus and Poisson’s ratio were determined from the strain field in the deformed configuration. In the same manner, the shear modulus was predicted from the shear deformation associated with the applied shear stress. The properties of the single graphene layer were then compared to those of the graphite flakes with multi-layers of graphene.

2. Molecular dynamics simulation

2.1. Construction of atomistic structures of graphite

Graphite structure is constructed by the carbon layers where the carbon atoms are arranged in a hexagonal pattern. The interatomic distance between the adjacent carbon atoms is 1.42 Å, and the associated atomistic interaction is covalently bonded by sp^2 hybridized electrons, the bond angle of which is 120° to each other. In naturally occurring or high quality synthetic graphite, the carbon layers are attacked along the thickness direction in AB type sequence with interlayer spacing of approximately 3.4 Å as shown in Fig. 1. Hereafter, the graphite with several carbon layers lumped together is referred to as graphite flakes. Because the adjacent carbon layers are held together by the weak van der Waals force, after proper processing [2,3], the stacked carbon layers can be dispersed and separated into a single layer that is usually called graphene sheet or graphene layer.

In order to investigate the mechanical properties of the graphite flakes and the graphene layer, the atomistic structures have to be constructed in conjunction with the appropriately specified atom-

istic interaction. In the description of graphite structure, two kinds of atomistic interactions are normally taken in account; one is bonded interaction, such as the covalent bond, and the other is the non-bonded interaction, i.e., van der Waals and electrostatic forces. Among the atomistic interactions, the covalent bond between two neighboring carbon atoms that provides the building block of the primary structure of the graphite may play an essential role in the mechanical responses. Such bonded interaction can be described using the potential energy that consists of bond stretching, bond angle bending, torsion, and inversion as illustrated in Fig. 2 [13]. Therefore, the total potential energy of the graphite contributed from the covalent bond is given as

$$U_{\text{graphite}} = \sum U_r + \sum U_\theta + \sum U_\phi + \sum U_\omega \tag{1}$$

where U_r is a bond stretching potential; U_θ is a bond angle bending potential; U_ϕ is a dihedral angle torsional potential; and U_ω is an inversion potential. For graphite structures under in-plane deformation, the atomistic interaction is mainly governed by the bond stretching and bond angle bending therefore, the dihedral torsion and inversion potentials that are related to the out-of-plane deformation were disregarded in the modeling. The explicit form for the bond stretching and bond angle bending can be approximated in terms of elastic springs as [14]:

$$U_r = \frac{1}{2} k_r (r - r_0)^2 \tag{2}$$

$$U_\theta = \frac{1}{2} k_\theta (\theta - \theta_0)^2 \tag{3}$$

where k_r and k_θ are the bond stretching force constant and angle bending force constant, respectively. The constants $k_r = 93,800 \frac{\text{kcal}}{\text{mole nm}^2}$ and $k_\theta = 126 \frac{\text{kcal}}{\text{mole rad}^2}$ selected from AMBER force field for carbon-carbon atomic-interaction [15] was employed in our molecular simulation. The parameters r_0 and θ_0 represent bond length and bond angle in equilibrium position, which are assumed to be 1.42 Å and 120°, respectively, for the graphite atomistic structures.

In addition to the bonded interaction, the non-bonded interaction between the carbon atoms was regarded as the van der Waals force, which can be characterized using the Lennard-Jones (L-J) potential as

$$U_{vdW} = 4u \left[\left(\frac{r_0}{r_{ij}} \right)^{12} - \left(\frac{r_0}{r_{ij}} \right)^6 \right] \tag{4}$$

where r_{ij} is the distance between the non-bonded pair of atoms. For the hexagonal graphite, the parameters $u = 0.0556 \text{ kcal/mole}$ and $r_0 = 3.40 \text{ Å}$ suggested in the literature [16] were adopted in the modeling. Moreover, the cutoff distance for the van der Waals force

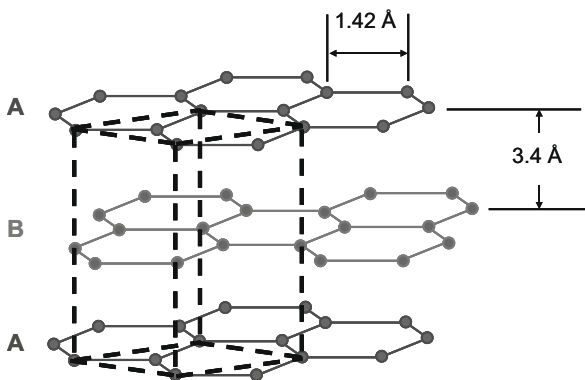


Fig. 1. Schematic of graphite structures.

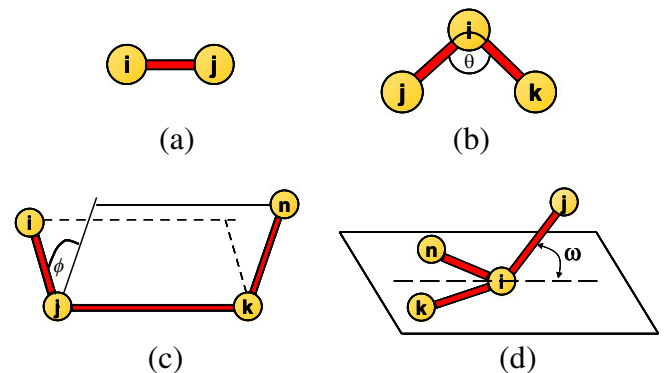


Fig. 2. A schematic of the inter-atomic potential: (a) bond stretch; (b) bond angle bending; (c) dihedral angle torsion; (d) inversion

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