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Effect of Graphene Sheets Aggregation on The Dislocation-Blocking Mechanism of Nanolaminated Aluminum/Graphene Composite: Molecular Dynamics Simulation Study

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ABSTRACT: Aluminum/graphene nanolaminated structures have a very proper reinforcing and toughening effect on aluminum composites. Graphene layers effectively prevent the growth and movement of dislocations in the aluminum matrix. Therefore, more and shorter dislocations lines occur in the aluminum matrix between the graphene layers. In this paper, tensile tests have been performed on nanolaminated aluminum/graphene composite using molecular dynamic simulation to study the dislocation-blocking mechanism and its reinforcing and toughening effect. The nucleation, expansion, and displacement of the dislocation in the aluminum matrix were investigated under tension. The results showed that the reinforcement mechanism includes increasing displacement density and shear stress transfer. Besides, the reinforcing and toughening effects were investigated as a function of the distance between the graphene sheets (the spacing of sheets between 4-14 Å). The results showed that the distance between the graphene sheets has an effective role in creating the dislocation-blocking mechanism in the aluminum matrix. Decreased graphene sheets increase the mechanical properties of the aluminum matrix due to the dislocation-blocking mechanism, which can be limited by the onset of graphene sheet aggregation. As the result, stable steps in 10-12 Å distance between graphene sheets were obtained by dislocations with a yield strength of about 14 GPa and yield strain of 0/065.

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1. INTRODUCTION

The strength efficiency of composites is strongly influenced by the way the reinforcing agent is placed in them [1]. Biological materials in nature, such as pearls, have high toughness and fatigue resistance due to their laminated structure. These properties have led researchers to use laminated nanostructures as reinforcements for the development of aluminum/graphene nanocomposites [2]. These features include two-dimensional structure, high specific surface area, and high modulus. In addition, aluminum layers limit the outward displacement of graphene, while graphene layers limit the displacement of the aluminum base. This significantly enhances the mechanical properties of the composite [3].

Recently, Zhou et al. [4] investigated the effect of graphene plate spacing on the properties of aluminum laminated composite. The results showed that reducing the distance between the plates due to the dislocation-blocking mechanism increases the mechanical properties of the composite. However, the optimal spacing of graphene sheets and the role of their aggregation on the properties of aluminum laminated composite have not been investigated so far.

In this study, to investigate the effect of aggregation of graphene plates on the properties of aluminum, the tensile properties of aluminum/graphene composite at different distances from graphene layers have been studied and evaluated using Molecular Dynamics (MD). For this purpose, parallel graphene plates were placed at specific intervals in the matrix of aluminum metal and the tensile test was applied perpendicular to the graphene plates.

2. SIMULATION METHOD

MD simulations were performed to fabricate aluminum/graphene composites using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software. In the early models, aluminum atoms were considered in a Face-Centered Cubic (FCC) structure with a grid size of 4/55 Å and graphene plates without any defects. Accordingly, the simulation model contains about 50,000 aluminum atoms and 5,000 carbon atoms. The configuration size of the simulation model was 7×9×15 nm^3. Graphene plates measuring 5×9 nm^2 were placed on an aluminum matrix. The volume percentage of graphene in the composite was considered to be 4%. The interaction between aluminum atoms was modeled using the potential of the Embedded Atom Model (EAM) [5]. The Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential was also used to model graphene plates [6]. In addition, van der Waals forces were modeled using the Leonard-Jones potential function [7].

As shown in Fig. 1, the tensile test is applied horizontally (in a *y*-direction) to the specimens. To prepare the simulation

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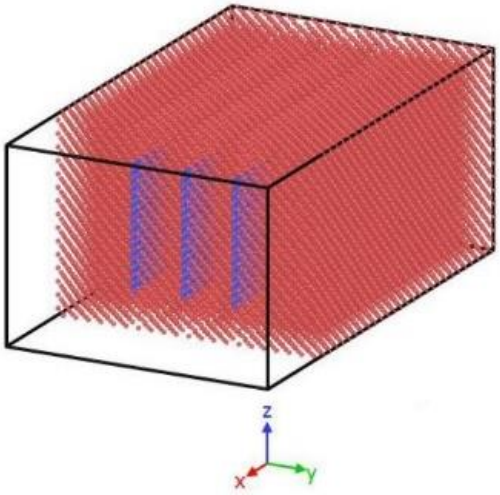

Fig. 1. Nanolaminated aluminum/graphene composite under tensile load in the y-direction.

structure, first, the whole system was subjected to energy minimization by conjugate gradient method by periodic conditions. Then, the process of thermodynamic optimization under NVT and NPT ensembles was performed based on Nose/Hoover thermostat and Nose/Hoover isobaric-isothermal ensemble at zero pressure at 300K for 100 ps. The time steps were set to 0/001 ps. In MD models, the microstructure is optimized when the potential energy of the system is balanced. Then, a uniaxial tension in the direction of the *y*-axis was applied by gradually expanding (pulling) the simulation box at a strain rate of 10^8 s^{-1}. Boundary conditions were assumed to be periodic in the direction of *x* and *z* and the direction of free tension. After the simulations, the Dislocation Extraction Algorithm (DXA) was used in OVITO software to detect and analyze the movements of the dislocation in the deformed structures [8].

3. RESULTS AND DISCUSSION

Fig. 2 shows the stress-strain diagrams of the specimens under tensile load for different spacing of graphene plates. By reducing the distance between the graphene plates from 14 to 10 Å, the elastic range increases by 13%, and the plastic deformation occurs at a higher strain (0065/). This trend is seen at intervals of 10-14 Å of graphene plates and the yield strength of the material increases by 30%.

Dislocations can be seen in Fig. 3 appearing inside the aluminum in addition to creating an interface. Dislocations are not able to penetrate the interface so the plastic deformation is limited in each of the aluminum layers. Dislocations are cut by graphene and accumulated in the interface. At distances less than 10 Å, graphene plates tend to accumulate graphene plates due to the gravitational force of van der Waals. As a result, the specific surface area available for graphene is reduced. At these distances, the graphene surface has less ability to cut dislocation. In the distances of 4-8 Å graphene plates, a reduction of the dislocations cut in the interface of graphene and aluminum can be observed, which has reduced the length of the dislocations. The composite has more in common between the 10 and 12 Å plates, which further locks the dislocations. Therefore, the propagation of dislocations

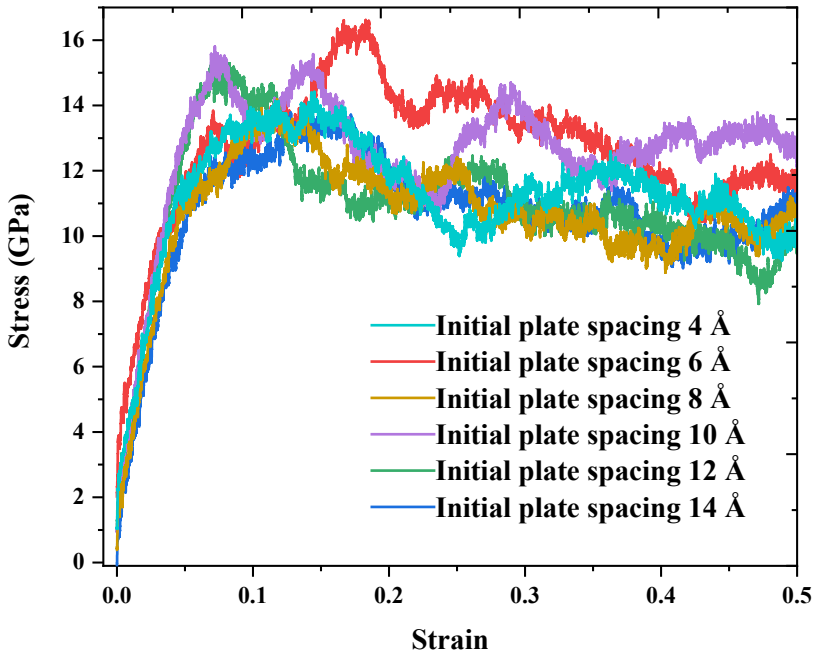

Fig. 2. Stress-strain diagram of aluminum/graphene composite.

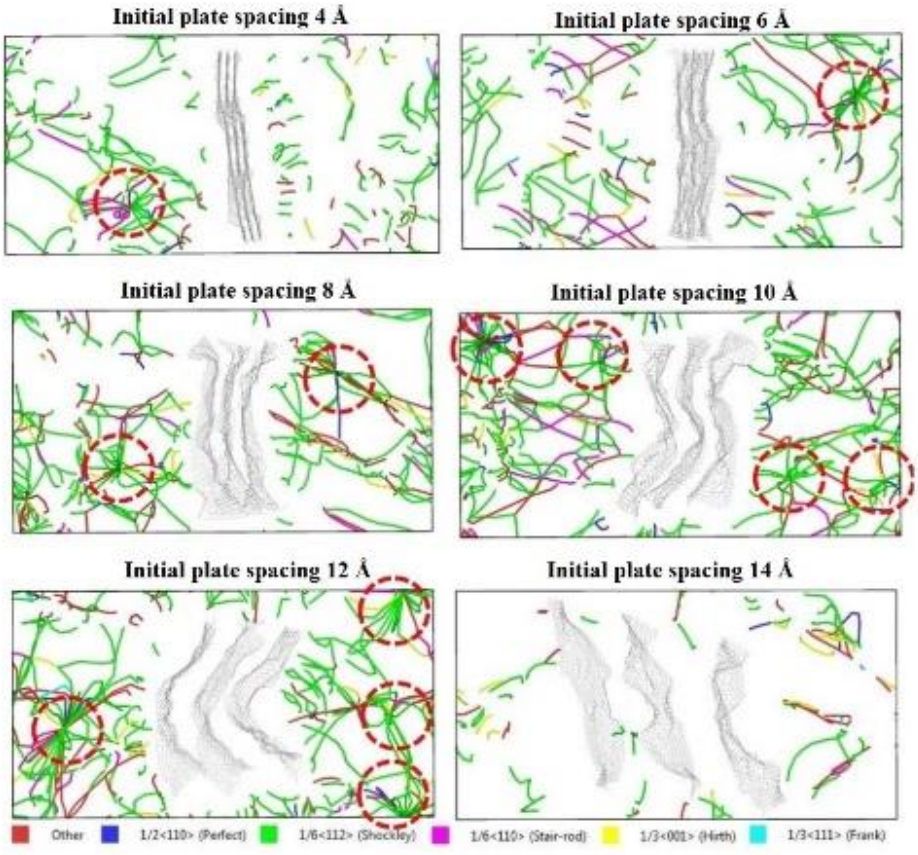

Fig. 3. Dislocation of nanolaminated aluminum/graphene composite in strain 0/12. The red dashed circles indicate dislocation-blocking.

becomes very difficult for composites with a plate spacing of more than 10 Å, which improves the mechanical properties of the aluminum/graphene composite. On the other hand, for the composite sample, the number of dislocation cuts in the graphene-aluminum interface has been reduced due to the influence of dislocation in the interface. Only low dislocation lengths can be observed in the interface of this sample. Such behavior has reduced the yield stress in this sample. As a result, the distance between the graphene plates in an optimal state (in this study 10 and 12 Å) can have the highest yield stress. This indicates that plate spacing and graphene aggregation have a significant effect on the dislocation-blocking mechanism. Due to the presence of graphene layers that can effectively block the dislocation, high engagement dislocations can be found in the samples. Therefore, the composites show high tensile strength, especially at intervals of 10 and 12 Å.

4. CONCLUSIONS

In this study, the mechanical properties of nanolaminated aluminum/graphene composites during uniaxial tensile application were investigated and evaluated using MD simulations. The results of the study are as follows:

1) Displacement slip is restricted and accumulated by graphene layers in nanolaminated aluminum/graphene composites and leads to increased displacement density in the interface.

2) Nanolaminated aluminum/graphene composites have higher yield strength and yield strain due to an increase in displacement density, decrease in plastic strain rate, and surface stress transfer effect. This increases the load-bearing capacity and flexibility of the composite.

3) The mechanism of dislocation-blocking shows a remarkable effect: nanolaminated aluminum/graphene composites perform better by reducing the distance between the plates. This is limited to intervals of less than 10 Å of graphene plates due to the aggregation of graphene plates. As a result, there is an optimal limit for graphene plates, which in this study was 10-12 Å.

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