Interaction Between Edge Dislocation and Single-Layered Graphene in Aluminum Matrix Investigated by Molecular Dynamics Simulation

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Abstract. The influence of graphene on dislocation movement and subsequent mechanical response of aluminum is investigated by the computational method of molecular dynamics simulation. A Lennard–Jones potential describing Al–C interaction was obtained through ab initio calculation. It was observed that the 2D graphene could reinforce Al matrix similar to the traditional Orowan mechanism. The Al/graphene interface first attract the gliding dislocation to reduce the system energy, which is unlike the grain boundary to repel gliding dislocations through pile-up mechanism. With the increase of stress, dislocation attracted and trapped at the front of graphene could glide along the interface and finally bypass it through climbing when graphene is orientated out of the shear plane. In addition, the strengthening ability of graphene is size dependent, showing a linear relationship between strength increment and graphene size.

Keywords: Graphene, Aluminum, Molecular Dynamics, Computational simulation.

1. Introduction
Metal-matrix composites always exhibit attractive mechanical properties as compared with their individual components [1]. However, the strength enhancement is always followed by a great ductility loss. The development of graphene has shed a light on the solution to this issue for engineers in academic and industrial fields [2,3]. This 2D material has a high strength and remains stable in matrix at higher than 1000 K [4]. Many investigations have shown the feasibility of graphene to tailor the mechanical and thermal properties of polymers, metals and their alloys [3,5].

The graphene reinforced metal-matrix composite (GRMMC) could be fabricated using powder metallurgy, physical/chemical vapor deposition, electrodeposition and so on [6]. These studies from literature have shown various properties, which makes the influence of graphene on mechanical behavior not well understood [7], e.g., the interaction mechanism between dislocation and graphene layer, the orientation and size dependence of strengthening. However, there are limited studies regarding the microscopic process during deformation.

In present study, a computational method of molecular dynamic simulation was used to investigate the interaction between edge dislocation and single graphene layer embedded in aluminum matrix during pure shear deformation. Graphene size and orientation have also been considered in order to elucidate their effects on the interaction mechanism and to evaluate the contributions to mechanical strength.
2. Simulation Methods
Molecular dynamic (MD) simulations were performed using LAMMPS (Large-scale atomic Molecular Massively Parallel Simulator) at constant temperature (0 K) and pressure (NPT). The initial dimension of simulation box is $359.4 \times 386.1 \times 128.6$ nm$^3$ with about 1.1 million Al atoms and a single-layered graphene with circular or square geometry, as shown in Fig. 1a. An edge dislocation was generated using displacement field before relaxation. The diameter and orientation were changed to investigate their influences on interaction behavior.

The EAM and Tersoff potentials [7,8] were used to compute the pairwise interactions of Al‒Al and C‒C, respectively. The 12‒6 Lennard‒Jones (LJ) type of van der Waals interaction was taken to describe the interfacial interaction of Al‒C. The well depth and equilibrium distance parameters in LJ potential were obtained by reproducing the quantum mechanical interaction energy curve from the dispersion corrected density functional theory calculations (Fig. 1b).

3. Results
3.1 Atomic Microstructure
Fig. 2 shows the interaction where the graphene normal to $[\,1\,1\,0\,]$ has a diameter of 51.4 nm. Simulation was started with an extended edge dislocation dissociated into two Shockley partials on (111) glide plane. As shown by the X-Y plane snapshots in Fig. 2a, the dislocation is obstructed firstly and then bypasses the graphene during shear. At 0.76% shear strain, the center part of dislocation begins to contact with the graphene, followed with a narrowing of stacking fault which nearly disappears at 0.9%. The corresponding X-Z plane snapshots in Fig. 2b exhibit that the bypassing process proceeds with downward climbing along $\langle\,1\,1\,2\,\rangle$ plane. The arrow marks a small step generated during bypassing.
Figure 2. Interaction of dislocation with circular graphene parallel with (1\bar{1}0) plane showing the pinning of the dislocation and subsequent bypass process

Fig. 3 shows the interaction when graphene is parallel with (111). Fig. 5a exhibits the obstruction similar to Orowan mechanism and a dislocation loop was left around the graphene. Fig. 5c demonstrates no climbing occurred in this case. The arrow refers to the attraction of dislocation by graphene.

Figure 3. Interaction of dislocation with graphene parallel with (111) showing the attraction and pinning of dislocation by graphene and subsequent bypass

Fig. 4 shows the interaction with a square graphene parallel with (1\bar{1}0). Fig. 4a exhibits the attraction of dislocation with graphene at first (open arrow), and bypass finally (dashed arrow line). However, bypass is hardly operated by climbing along [111]. Instead, one of the dislocation arms could move towards the other one when strain is higher than 0.98%, and finally combine together before escaping out the crystal. A slight climbing of one arm was observed (solid arrow).
3.2 Mechanical Behaviour

Fig. 5 shows the mechanical performance with and without graphene related to Fig. 2. Shear stress–strain curves are exhibited in Fig. 5a, where the stress begin to drop beyond 0.5% strain due to the escape of dislocation out of the boundary. Compared with the microstructure evolution in Fig. 2, four stages are clear in Fig. 5b. Dislocation move towards graphene initially, followed by stress drop due to attraction (Stage A). While the dislocation is obstructed by graphene, the arms could glide ahead continuously, followed by a sharp stress rise (stage B). Further shear causes dislocation climbing (stage C), and then escape out of the box (Stage D). More cases with different graphene diameter but the same orientation are shown in Fig. 5c.

Fig. 6a shows the strengthening ability of square graphene with different area, which is similar to the circular graphene, but with a bit longer stage C due to constant bypass length with climbing. Fig. 6b demonstrates strengthening dependence on graphene orientation, showing clearly different attraction and pinning abilities.
4. Discussion

The discussion focus on the strengthening model of GRMMCs. The simulation results demonstrate that the shear stress required to bypass over the graphene normal to shear direction depends closely on its size for both circular and square graphene. When the diameters have increased from 25.7 nm to 115.7 nm, the peak values indicating the shear resistance introduced by single-layered graphene increase from 10 MPa to 92 MPa. Orowan strengthening mechanism have been observed in present study. This strengthening capacity depends on the particle size and inter-particle spacing, which could be estimated by Ashby’s model [9],

$$\Delta \sigma = \frac{Gb}{2.38\pi(1-\nu)^{1/2}} \ln\left(\frac{d}{2b}\right)$$

where G is the shear modulus (26 GPa for Al), b the magnitude of Burgers vector (0.2864 nm for Al), \(\nu\) the Poisson’s ratio (0.35 for Al), L the effective spacing between graphene layers (note the simulation box has periodic boundary), and \(d\) the diameter or width of graphene. As the boundary of simulation box along Y direction is periodic, L and \(d\) has a relation of \(L+\frac{d}{2}=386.07\) nm.

Based on Ashby’s model in the equation (1), the increment of shear stress due to obstruction of graphene is proportional to a dimensionless variable \(\frac{b}{L} \ln\left(\frac{d}{2b}\right)\). Fig. 7a shows the linear relationship between stress increment and this variable, which exhibits a slope of 24.3 GPa. Compared with Ashby’s prediction of 4.3 GPa, the slope indicating the ability to obstruct dislocation movement is increased significantly GRMMCs, which is in line with literature reports [3,10].
5. Conclusions

MD simulation was carried out in this study to investigate the interaction between an edge dislocation and a single-layered graphene in Al matrix under pure shear deformation. The main conclusions are addressed as follows:

(1) The *ab initio* calculation results show an van der Waal’s type interaction for Al-C atoms, and the depth of interaction ($\varepsilon$) and the radius ($\sigma$) of 12-6 LJ potentials are obtained as 0.005 eV and 3.576 Å.

(2) Two bypass mechanisms were observed. When graphene size along climb direction is small, dislocation could bypass the graphene through climbing mechanism. Otherwise, dislocation would surround the graphene and leave a dislocation loop. No shear fracture of graphene was observed.

(3) The stress increment attributed to graphene shows a linear relationship with graphene size, which could be interpreted by Ashby’s model regarding the linearity, but with a larger hardening coefficient than prediction.

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