Anisotropy Behavior of Dislocation Nucleation from a Sharp Corner in Copper*

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Abstract

By means of reaction pathway analysis, we have investigated the nucleation of 90° and 30° partial dislocation from a sharp corner in an f.c.c. crystal copper. The anisotropy aspects of dislocation nucleation revealed by the results have shown that the stress-dependent activation energy of 30° partial dislocation is approximately twice over the counterpart of 90° partial dislocation, and that the maximum inelastic displacement for the former is also higher. Moreover, the shape of the saddle-point configuration of 30° partial dislocation is similar to a half-ellipse whereas in the case of 90° partial dislocation it is more like a semi-circle, reflecting the different Peierls barriers influenced by the Burgers vectors. Further study of the surface reconstruction demonstrates that although the nucleation of 30° partial dislocation has been enhanced by surface reduction, it is still more energy-unfavorable than the 90° partial dislocation. These results suggest that the higher Peierls barrier is responsible for the larger activation energy of 30° partial dislocation nucleation.

Key words : Dislocation Nucleation, Reaction Pathway Analysis, Molecular Dynamics, Copper, Anisotropy Behavior

1. Introduction

Since the recent establishment of greater requirements for using metallic elements at a sub-micron scale, dislocation nucleation at free surface and stress concentrations has begun to attract more attention with regard to the role it plays as a governing factor in macroscopic behavior^{(1)–(3)}.

Previously, many researchers have focused on dislocation emissions in nanostructured metals so as to probe the implications of brittle versus ductile behavior of crystalline materials based on the Peierls concept⁽⁴⁾, atomistic simulation^{(1),(5),(6)}, and multiscale models⁽⁷⁾. Recently, Zhu *et al.* described the emissions of an embryonic dislocation loop from a stressed crack tip in copper with full atomistic details. They have reported the saddle-point configuration and activation energy for the nucleation of 90° partial dislocation via reaction pathway sampling schemes. Based on a similar framework, Boyer explored the stress-dependent behavior of dislocation nucleation in a homogeneous system and from a heterogeneous source of point defects, vacancy clusters, and nanowire surfaces in copper from both structural and energetic perspectives⁽⁸⁾. This approach has also been successfully applied to various materials involving dislocation nucleation processes, such as in research regarding a shuffle-set dislocation loop from a sharp corner in silicon⁽⁹⁾ as well as a comparison with glide-set⁽¹⁰⁾, and dislocation nucleation from a surface step in nickel⁽¹¹⁾.

However, in terms of the anisotropy aspects of dislocation nucleation, although the generalized Peierls-Nabarro models have made some efforts to introduce full elastic anisotropy^{(12),(13)}, there has been a lack of information supplied by atomistic simulation with regard to this issue. In the present work, we performed reaction pathway analysis^{(6),(9),(11)} of two partial dislocations from a sharp corner in copper to investigate anisotropy effects dependent on dif-

ferent Burgers vectors. In such a close-packed lattice, the perfect dislocation dissociates into two Shockley partial dislocations connected by a stacking fault and shows complex behavior in dislocation nucleation and emission processes⁽¹⁴⁾. And due to the two possible directions of the Burgers vectors along the $\langle 112 \rangle$ direction, which correspond, respectively, to 90° and 30° partial dislocation, the question arises as to how the orientations influence the dislocation nucleation. Several researchers have numerically characterized the anisotropy aspect of dislocation nucleation by nanoindentation, demonstrating that copper with a larger anisotropy factor shows a dramatic anisotropy effect^{(15), (16)}, these studies, however, only focused on different crystallographic surfaces.

To our knowledge, there has been no research regarding the anisotropy behavior of dislocation nucleation dependent on different slip orientations from a sharp corner in copper. Thus, we devoted our attention to illustrating the Burgers vector effects on activation energies and the saddle-point configurations of partial dislocation nucleation, with the purpose of obtaining a valuable and novel understanding of the anisotropy aspects of dislocation nucleation.

2. Simulation methods

Fig. 1 Schematic of the dislocation nucleation model. The two arrows on the $(\bar{1}\bar{1}1)$ slip plane show the directions of two partial dislocations. Periodic boundary conditions are applied in all three directions. The simulation cell and the corners have been illustrated on the right.

The computational model is schematically shown in Fig. 1. A sharp corner was formed by removing 1/3 of the cell size along the x and z axis in a single crystal copper. Periodic boundary conditions were imposed in all directions. The system size was $15.3 \times 7.7 \times 15.2 \text{ nm}^3$ and included 140 280 atoms. The interaction between copper atoms was described by the Mishin potentials⁽¹⁷⁾. With a time step of 0.54 fs, the Molecular Dynamics (MD) simulations were conducted with the Verlet method, which is a numerical technique used to perform integration of motion equations⁽¹⁸⁾. In order to study the anisotropy effects of these two different Burgers vectors according to 90° partial dislocation ($\vec{b}_{90P} = a_0/6[\bar{1}\bar{1}2](\bar{1}\bar{1}1)$) and 30° partial dislocation ($\vec{b}_{30P} = a_0/6[\bar{2}1\bar{1}](\bar{1}\bar{1}1)$) ($a_0 = 0.362 \text{ nm}$), pure shear stress was applied to two slip systems, $[\bar{1}\bar{1}2](\bar{1}\bar{1}1)$ and $[\bar{2}1\bar{1}](\bar{1}\bar{1}1)$, respectively, which meant that the resolved shear stress along these two slip directions was maximized. Since the stress field was inhomogeneous near the sharp corner, we used the nominal resolved shear stress calculated without considering the effect of a square hole. By transforming the applied stress value to the strain tensor according to elastic theory, we calculated the shape matrix of the simulation cell after deformation and

loaded the system by changing the cell shape⁽⁹⁾. The MD simulation has been done under constant low temperature (0.001 K) to avoid or minimize the aid of thermal fluctuation, with the purpose of approximately evaluate the athermal stress.

Then the reaction pathway analysis has been performed by nudged elastic band (NEB) method to obtain the activation energy barriers and saddle-point configurations under various stress levels. The input of NEB method is an initial guess of the energy pathway composed of a string of images. Each of the images corresponds to a specific state and geometry of the atoms, a snapshot along the reaction path. As the convergence of the NEB method is greatly affected by the initial guess of the energy pathway, it is very important to determine the string of images as input. For each NEB calculation of the two partial dislocations, we inserted a partial dislocation loop based on dislocation theory and then unloaded this cell by MD simulation under constant low temperature (0.001 K)⁽⁶⁾. The input pathway of NEB calculation, including 20 atomic configurations, was picked up from the snapshots of the unloading result.

For a range of stress levels at a given τ , we have utilized the NEB method and incorporated various techniques, including the improved tangent method⁽¹⁹⁾, the climbing image method⁽²⁰⁾, and the free-end method⁽²¹⁾, to carry out the calculation and to induce the convergence, which was determined as the potential force on each replica vertical to the path becomes less than 0.005 eV/Å.

3. Results and discussion

Fig. 2 Dependence of activation energy on shear stress for the nucleation of two partial dislocations.

The magnitude of the Burgers vectors is the same for both 90° and 30° partial dislocations, $b_p = a_0 / \sqrt{6} = 0.148$ nm. However, the stress-dependent activation energy of 30° partial dislocation is approximately twice the counterpart of the 90° partial dislocation, shown in Fig. 2, which means that 30° partial dislocation nucleation is energy-unfavorable compared to the 90° partial dislocation. The dependence of activation energy on applied shear stress can be fitted by empirical formula $\Delta E = A(1 - \tau/\tau_{ath})^n$, $A = 8.9$ eV, $n = 1.90$ and $\tau_{ath} = 1.67$ GPa for 90° partial, whereas $A = 17.9$ eV, $n = 2.32$ and $\tau_{ath} = 1.88$ GPa for 30° partial can be obtained. The exponent n is similar between the two cases and also close to the case of homogeneous nucleation ($A = 13.7$ eV, $n = 1.82$)⁽⁸⁾ and nucleation from vacancy ($A = 14.3$ eV,

$n = 1.94$)⁽⁸⁾ in copper. Nevertheless, the prefactor A of the 30° partial dislocation is twice that of the 90° , and both are much lower than that of nucleation from a sharp corner in the shuffle-set of silicon ($A = 111.5$ eV, $n = 1.87$)⁽⁹⁾. The unstable stacking fault energies (γ_{us}) of copper and silicon calculated by the corresponding interatomic potentials (Mishin potential and SW potential) are 0.16 J/m² and 0.83 J/m², respectively, reflecting the lower energy barrier of metallic bonding.

Fig. 3 Maximum inelastic displacement of the saddle-point configurations for the nucleation of two partial dislocations.

Reasonably, the maximum inelastic displacements, which are defined by the length of the slip vector⁽²²⁾, as shown in Fig. 3, have also exhibited a higher value with 30° partial dislocation. The inelastic displacement given by the slip vector provides us with the total magnitude of the slip for atoms between two adjacent planes while ignoring the directions. Hence, it is not identical to the Burgers vector, especially with regard to the displacement orientations and its ability to provide a clear description of the core field properties. However, comparing with Fig. 2 and Fig. 3, it is clear that under the same shear stress value, 30° partial dislocation creates greater displacement between the adjacent slip layers and accordingly requires more activation energy. Our results suggest that the higher stress-dependent activation energy of the 30° partial dislocation nucleation is primarily due to its larger inelastic displacement.

Additionally, the saddle-point configurations visualized by slip vector have been depicted in Fig. 4. The shapes and relative displacement distribution profiles are also different from each other. The loop of the 90° partial dislocation seems more like a semi-circle, while the shape of the saddle-point configuration of the 30° partial dislocation is similar to a half-ellipse, and the distinction is more remarkable within the larger saddle-point configuration loops under low stress. The inhomogeneous stress field within the area swept by the dislocation presents higher value near the corner while the middle point of dislocation line far from the corner is exerted under lower stress, which could restrain both of the two partial dislocations from extending along the direction perpendicular to the sharp corner. Furthermore, the different mobility of edge, screw, and 30° component along the dislocation line of the two partial dislocations, as indicated by the arrows shown in Fig. 4, could also play a role of the shape difference. Both the Peierls model and atomistic simulation have indicated that the Peierls

Fig. 4 Various saddle-point configurations of the two partial dislocation nucleations under various stress values from a sharp corner viewed by slip vector. The Burger's vector as well as the edge, screw, and 30° components have been shown in the first image of both cases: (a) 90° partial dislocation and (b) 30° partial dislocation.

energy of the edge component is much lower than that of the screw component, and that the mixed 30° is intermediate, which correlatively contributes to the different mobility properties (Peierls energy: screw $>$ 30° $>$ edge, mobility: edge $>$ 30° $>$ screw)^{(23), (24)}. For the 90° partial dislocation loop which has screw components at two edges (Fig. 4 (a), arrow a1 and a2) and edge component at the middle (Fig. 4 (a), arrow a3), it is easier for the edge part to move than the screw part, so the middle of 90° partial moves faster. Balanced with the inhomogeneous stress effect mentioned above, the dislocation line shows approximately a semi-circle shape. Nevertheless, the shape of the 30° partial dislocation appears to be a half-ellipse since the edge component is located on the left (Fig. 4 (b), arrow b1) and promotes movement of the loop towards the left end. The edge component always dominantly controls the movement of dislocation, thereby influencing the shape of the dislocation line because of its higher mobility. Theoretically, the widest dislocation core width of edge component among these three could be the basic origin of the differences in Peierls energy as well as the mobility⁽²⁵⁾ and lead to the relevant characteristics of geometrical anisotropy features of dislocation in this result. In addition to controlling the dislocation-loop shape, the lower Peierls barrier of the edge component could enhance the 90° partial dislocation nucleation and accordingly result in lower activation energy. However, since the dislocation nucleation occurs at an atomic level, it is beyond the scale of dislocation theory and can only be investigated by the atomic simulation, such as the framework shown here. By means of the explanations via Peierls energy which is the evaluation for dislocation mobility, we could only provide the qualitative rather than quantitative interpretation for the results of our simulation on dislocation nucleation.

In order to discuss the difference in activation energy between these two partial dislocations, we have also examined the surface reconstruction of the sharp corner in the present system. Fig. 5 provides the relative displacement of the atoms located on the tip of sharp corner with respect to the adjacent slip layer. Following the atomic view at the top right of Fig. 5, the positive value of displacement means the reduction of the surface area and the larger value illustrates more energy reduction. It is found that both the 90° and 30° partial dislocation nucleation processes decreased the surface energy by surface reduction. However, since the displacement of atoms is larger in the case of 30° partial dislocation nucleation, as shown in Fig. 5, the reduction of surface energy resulting from the 30° partial dislocation is

Fig. 5 Displacement of the atoms located on the tip of sharp corner relative with the adjacent slip layer under resolved shear stress of 1.3 GPa. The coordination equals to the y axis in the simulation model shown in Fig. 1. Both of the relative displacement and coordination have been normalized by the magnitude of the Burgers vector of partial dislocations, b_p .

even more than that from the 90° partial. As comparing with the activation energy of dislocation nucleation process, we therefore must declare that although the surface reduction ‘helps’ with the nucleation process of 30° partial dislocation to some extent, it still occurs with more difficulty than with the 90° partial dislocation. Consequently, it is assumed that the Peierls barrier rather than the surface effect accounts for the difference in activation energy during the dislocation nucleation process in the present results.

4. Conclusions

The anisotropy effects of dislocation nucleation have been researched by reaction pathway analysis on nucleation of two partial dislocations from a sharp corner in copper. The results have shown that the activation energy of 30° partial dislocation is nearly twice that of 90° partial dislocation, and that the maximum inelastic displacements of saddle-point configurations are also greater in the former. Furthermore, the loop shape of 90° partial dislocation seems more like a semi-circle, whereas in the case of 30° partial dislocation it is similar to a half-ellipse, which could be principally ascribed to the Peierls barrier differences between edge and screw components and the inhomogeneous stress field. By means of the results, we speculate that the Peierls barrier also plays a role in the dislocation nucleation process and has an impact on the required activation energy. We believe that the anisotropy aspect of dislocation nucleation exhibited by our simulation provides useful insight into the incipient plastic deformation of nanoscale metals.

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