1022 Dislocation nucleation from a sharp corner in copper: Difference between 90° partial and 30° partial

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I. INTRODUCTION

Since the larger requirements of metallic elements with submicron scale recently, dislocation nucleation at free surface and stress concentration has attracted even more attention, for the role of which plays as a governing factors of macroscopic behavior^{1,2,3}.

Previously, many researchers have focused on the dislocation emission from a stressed crack tip in nanostructured metals so as to demonstrate the implications on brittle versus ductile behavior of crystalline materials by means of the Peierls concept⁴, atomistic simulation^{1,5,6} and multiscale model⁷. Recently, Zhu et al. have obtained a description of the emission of an embryonic dislocation loop from a stressed crack tip in copper by full atomistic details. They have reported the saddle-point configuration and activation energy for the nucleation by using reaction pathway sampling schemes. This approach has been successfully applied on various models involving dislocation nucleation processes, such as a sharp corner of silicon⁸ and a surface step in nickel⁹.

However, in terms of anisotropy aspects of nucleation, although the generalized Peierls-Nabarro models have made some efforts to introduce the full elastic anisotropy^{10,11}, there is a lack of information supplying by atomistic simulation on this issue. In the present work, we performed an atomistic calculation based on Zhu's framework to two partial dislocations from a sharp corner in copper to investigate the anisotropy effects depending on different Burgers vectors.

II. SIMULATION METHODS

FIG. 1 Schematic of the dislocation nucleation model. The two arrows on $(\bar{1}\bar{1}1)$ slip plane show the directions of two partial dislocations.

Consider a sharp corner in a single crystal Cu, which was made by removing 1/3 of the cell size along x and z axis, schematically shown in Fig. 1. Periodic boundary conditions were imposed in all directions. The system size was $153.4 \times 76.7 \times 151.8 \text{ nm}^3$ and included 140 280 atoms. The interaction between Cu atoms was described by Mishin potentials¹². Molecular Dynamics (MD) simulations were conducted with Verlet method according to a time step of 0.54 fs. 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, in order to study the anisotropy effects of these two different Burgers vectors according to 90° partial dislocation ($\mathbf{b}_{90p} = a_0/6[\bar{1}\bar{1}2](\bar{1}\bar{1}1)$) and 30° partial dislocation ($\mathbf{b}_{30p} = a_0/6[\bar{2}1\bar{1}](\bar{1}\bar{1}1)$) ($a_0 = 0.362 \text{ nm}$).

For a range of stresses at a given τ , the NEB method has been utilized to achieve the minimum energy pathway for two partial dislocations respectively. Besides, various techniques, including the improved tangent method¹³,

climbing image method¹⁴ and free-end method¹⁵, have been incorporated and combined to do the calculation and to induce the convergence which is judged as the potential force on each replica vertical to the path becomes less than $0.005 \text{ eV}/\text{\AA}$.

III. RESULTS AND DISCUSSIONS

FIG. 2. Dependence of activation energy on shear stress for the nucleation of two partials. The solid lines are fitted by the form of $\Delta E = A(1 - \tau/\tau_{\text{ath}})^n$.

FIG. 3. Maximum inelastic displacement of the saddle-point configurations for the nucleation of two partials.

The magnitude of the Burgers vectors is same for both 90° and 30° partial dislocations, $b_p = a_0/\sqrt{6} = 1.476 \text{\AA}$. However, the stress-dependent activation energy of 30° partial dislocation is approximately twice over the counterpart of 90° partial dislocation, shown in Fig. 2, which means that 30° partial dislocation nucleation is energy unfavorable than 90° partial. The dependence of activation energy on applied shear stress can be fitted by empirical formula $\Delta E = A(1 - \tau/\tau_{\text{ath}})^n$, and $A = 8.9 \text{ eV}$, $n = 1.90$, and $\tau_{\text{ath}} = 1.67 \text{ GPa}$ for 90° partial, whereas $A = 17.9 \text{ eV}$, $n = 2.32$, and $\tau_{\text{ath}} = 1.88 \text{ GPa}$ for 30° partial can be obtained.

The exponent n is similar with each other and also similar to the case of homogeneous nucleation ($A = 13.7 \text{ eV}$, $n = 1.82$)¹⁶ and nucleation from vacancy ($A = 14.3 \text{ eV}$, $n = 1.94$)¹⁶ in copper. Whereas the prefactor A of the 30° partial is 1.5 times of the 90° , and both of them are much lower than that of nucleation from a sharp corner in the shuffle-set of silicon ($A = 111.5 \text{ eV}$, $n = 1.87$)⁸. The unstable stacking fault energy (γ_{us}) of copper and silicon calculated by the corresponding interatomic potentials (Mishin potential and SW potential) are 158 mJ/m^2 and 830 mJ/m^2 , respectively, reflecting the lower energy barrier of metallic bonding.

Reasonably, the maximum inelastic displacements, which are defined by the length of slip vector, shown in Fig. 3, have also exhibited higher value with 30° partial, which is a coincidence of the tendency on the activation energy between the two partials presented above. The inelastic displacement given by slip vector provides us the total magnitude of the slip for atoms between two adjacent planes while ignoring the directions. Hence, it is not exactly identical with the Burgers vector especially when concerning the displacement orientations and intending to obtain a clear description of core field properties. However, it has suggested that the higher stress-dependent activation energy of the 30° partial dislocation nucleation could be mainly attributed to its larger inelastic displacement.

a. Saddle-point configurations of 90° partial dislocation nucleation under various stress values. The Burger vector as well as the edge and screw components have been shown in the first image.

b. Saddle-point configurations of 30° partial dislocation nucleation under various stress values. The Burger vector as well as the edge and screw components have been shown in the first image.

FIG. 4. Various saddle-point configurations of the two partial dislocations from a sharp corner.

Besides, 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 90° partial dislocation seems more like a semi-circle whereas the shape of saddle-point configuration of 30° partial dislocation is similar to an oblate half-hexagon. The distinction could be primarily leading by the different Peierls barrier between edge, screw and 30° component located in different points along the two

partial curved dislocations, as shown in Fig. 4. Both of the Peierls model and atomistic simulation have reported that the Peierls energy of edge component is much lower than screw component and the mixed 30° one is mediate, leading to the higher mobility of the former, then the mixed 30° one and the screw dislocation is the lowest^{17,18}. Theoretically, the wider dislocation core width of edge dislocation, as the basic origin of difference on Peierls energy and mobility, could also be a crucial evidence of the analysis above¹⁹. The Burgers vector effect on dislocation core structure lead to the relevant characteristics of saddle-point configurations and activation energy, also elucidating the marked anisotropy features of dislocation nucleation phenomena in copper.

IV. CONCLUSIONS

The anisotropy effects of dislocation nucleation have been researched by reaction pathway analysis of the two partial dislocations nucleation from a sharp corner in copper. The results have shown that the activation energy of 30° partial dislocation is nearly twice of 90° partial dislocation and the maximum inelastic displacements of saddle-point configurations are also greater of the former. Moreover, 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 an oblate half-hexagon, which can be principally ascribed to the mobility differences. 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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