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Large scale atomistic simulations of screw dislocation structure, annihilation and cross-slip in FCC Ni

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Abstract

Using QM-Sutton-Chen many-body potential, we have studied the $1/2a\langle 1\,1\,0\rangle$ screw dislocation in nickel (Ni) via molecular dynamics (MD) simulations. We have studied core energy and structure using a quadrupolar dislocation system with 3D periodic boundary conditions. The relaxed structures show dissociation into two partials on $\{1\,1\,1\}$ planes. The equilibrium separation distance between the two partials is 2.5 nm, which is larger than the derived value according to experimental data, due to low stacking fault energy given by the QM-Sutton-Chen force field. From our calculations, the core energy for the $1/2a\langle 1\,1\,0\rangle$ screw dislocation is 0.5 eV/b. We also studied motion and annihilation process of opposite signed dislocations. We build the dipole system with two combinations of dissociation planes: (a) two dislocations dissociated on intersecting slip planes and (b) two on parallel planes. The process of cross-slip and associated energy barriers are also calculated from these simulations.

Keywords: Atomistic simulations; Dislocation; Molecular dynamics

1. Introduction

Dislocations are important factors in controlling the mechanical properties of ductile materials. Atomistic simulations can provide us with a detailed description which is beyond the scope of classic continuum dislocation theory. In fcc metals, the perfect screw dislocation, with Burgers vector $b = 1/2a\langle 1\,1\,0\rangle$, dissociates into two Schockley partials to lower the energy [1], the properties of these partials are dominant factors in the motion and interaction of dislocations.

Swaminarayan et al. [2] and Rasmussen et al. [3] studied the motion and annihilation of dislocations in copper from an atomistic point of view. Due to the dissociation of the perfect screw dislocation, different configurations of dislocation dipoles need to be considered; the process of dipole annihilation in Ni is main focus of this paper.

Cross-slip (where screw dislocations move from one slip plane to another one) is a fundamental factor in determining the mechanical behavior of metals, and it is related to the onset of stage III in the stress strain curve of single crystals. While perfect screw dislocation can cross-slip freely, the dissociated dislocations in fcc crystals require an external force to cross-slip due to the edge components of their partials. The classical theory requires the partials to associate into a perfect dislocation to cross-slip. The Friedel–Escaig [4,5] model of this constrain process states that on the primary slip plane, the partials must be recombined over a short length before the whole screw dislocation re-dissociates on the cross-slip plane. Recently, Rasmussen et al. [6] calculated the activation energy for cross-slip in copper from MD simulation, using a predetermined path for cross-slip. Duesbery studied two-dimensional rigid dislocations in copper with atomistic simulations [7]; he finds that cross-slip can occur without the constriction of the partials in the primary plane if the shear stress is large enough. We study the process of cross-slip in Ni using dislocation dipoles in a periodic simulation cell.

2. Computational method

We use the MpiSIM parallel MD code with the QM-Sutton-Chen many-body potential for Ni, which gives accurate values of elastic constants and surface energy [8–10].

In order to get relaxed core structure and energy, we build a dislocation quadrupole system in a simulation cell with 3D periodic boundary condition, in which there are two dislocations with Burgers vector $1/2a\langle 1\,1\,0\rangle$ and two with $1/2a\langle \bar{1}\,\bar{1}\,0\rangle$. We construct the screw dislocations using the displacements obtained from elastic theory and then all atomic positions are relaxed with energy minimization.

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We study dislocation motion, annihilation and cross-slip using a dislocation dipole in a periodic simulation cell. Since the screw dislocations can dissociate on two equivalent (1 1 1) planes, there are three configurations of the dipole: (a) the two dislocations dissociate on the same slip plane; (b) they dissociate on two intersecting slip planes and (c) on two parallel slip planes. Clearly, cases (b) and (c) are the most interesting since cross-slip is needed for the annihilation to occur; we will concentrate on these two cases. Our dipole simulation cells contains 22,050 atoms (15.03 nm along x direction and 9.11 nm along y direction). The distance of the centers of two opposite sign screw dislocations was 9 nm along x.

3. Results and discussion

3.1. Core structure and core energy

The total energy of a system containing dislocations can be divided into a term associated with the core of the dislocations and an elastic part, which can be calculated using linear elasticity theory. For our quadrupole system, if we consider the dislocations as not dissociated, the total energy can be written as [11]

$$E = E_c(r_c) + \frac{Kb^3}{4\pi}\left[\ln\left(\frac{d_1}{r_c}\right) + A\left(\frac{d_1}{d_2}\right)\right] \quad (1)$$

where E_c is the core energy and the second term is the elastic energy which contains self energies as well as interactions, K a constant related to the elastic constants, d_1 and d_2 the distance of two screw dislocation cores along x and y directions. The term $A(d_1/d_2)$ contains the sum of all dislocation interactions and depends on the geometry of the simulation cell; it can be evaluated numerically. Fig. 1 shows E/b as a function of $\ln(d_1/r_c) + A(d_1/d_2)$, for systems of different sizes, ranging from 11,760 to 105,840 atoms, and the separation between dislocations ranging from 2.8 to 12.9 nm. We can see that our atomistic results follow the straight line predicted by elasticity theory (Eq. (1)). From a linear fit, we find the core energy to be $E_c = 0.544\,\text{eV}/b$ and the elastic modulus $K = 44.64\,\text{GPa}$.

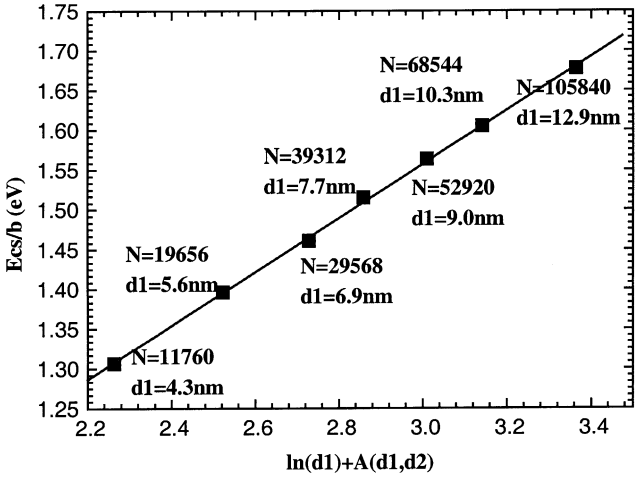

Fig. 1. Total energy as a function of $\ln[d_1/r_c + A(d_1, d_2)]$ for simulation cells of different sizes. The number of atoms in each simulation is shown.

Using our force field (FF) we can calculate the atomic energy associated with each atom. If we define the core as the six atoms with higher energy per partial, we obtain the core energy of each partial as $0.248\,\text{eV}/b$, which agrees well with the core energy we got from elastic method. The core shape of the partials is planar and its length is 5 Å along (1 1 1) plane.

We define the position of the partial as the atom with the highest energy in the core, which leads to the equilibrium distance of two partials of 25 Å. From elasticity theory, the distance separating the two partials is given by [12]

$$D_e = \frac{b^2(K_s - K_e)/3}{8\pi\gamma} \quad (2)$$

where K_s and K_e are anisotropic elastic energy factors for screw and edge components and γ the stacking fault energy. The calculated D_e is 15.25 Å based on our FF values ($C_{11} = 231.6\,\text{GPa}$, $C_{12} = 161.5\,\text{GPa}$, $C_{44} = 99.85\,\text{GPa}$, $\gamma = 40\,\text{mJ/m}^2$, $a = 3.46$ Å), less than the one obtained from the simulations. Similar behavior was found by Duesbery [7] and Rasmussen [6] in Cu.

3.2. Dislocation dipole annihilation: dissociation on intersecting planes

To study dislocation motion, annihilation and cross-slip, we build a dipole with dislocations dissociated on two intersecting planes, see Fig. 2a. When we have $1/2[1\,1\,0]$ dissociated on $(\bar{1}\,1\,1)$ plane, the reaction is $1/2[1\,1\,0] \rightarrow 1/6[1\,2\,1] + 1/6[2\,1\,\bar{1}]$, and $1/2\lfloor\bar{1}\,\bar{1}\,0\rfloor$ dissociated on $(\bar{1}\,1\,1)$ plane, the reaction is $1/2\lfloor\bar{1}\,\bar{1}\,0\rfloor \rightarrow 1/6\lfloor\bar{2}\,\bar{1}\,1\rfloor + 1/6\lfloor\bar{2}\,\bar{1}\,\bar{1}\rfloor$. Fig. 2 shows four snapshots of the annihilation process. We show differential displacement maps (DDM) where the atoms are projected on a (1 1 0) plane and the arrows represent displacements on a $\langle 1\,1\,0\rangle$ direction. From the DDM, we also see the core structure of each screw has a planar shape, and the atoms with highest energy are spread on (1 1 1) plane, with a planar shape as well. We can see that partial $1/6\lfloor\bar{1}\,\bar{2}\,1\rfloor$ (P3) moves on the $(\bar{1}\,1\,1)$ plane towards the other dislocation (partials P1 and P2). P1 and P2 have to cross-slip before annihilating with P3. From Fig. 2b and c, we can see that the distance between P1 and P2 diminishes as P3 approaches them. P1 and P2 dissociate into the other two partials, $1/6[2\,1\,1]$ and $1/6[1\,2\,\bar{1}]$. Annihilation then occurs between $1/6[\bar{1}\,\bar{2}\,1]$ and $1/6[1\,2\,\bar{1}]$ and the only partial left is $1/6[2\,1\,1]$. In Fig. 2d, we have two partials and a stacking fault in between. The screw dislocation $1/2\langle\bar{1}\,\bar{1}\,0\rangle$ crossed slip in order to annihilate with $1/2\langle 1\,1\,0\rangle$, since they were on different slip planes originally. In Fig. 2e, we show the total energy as a function of time; arrows mark the times

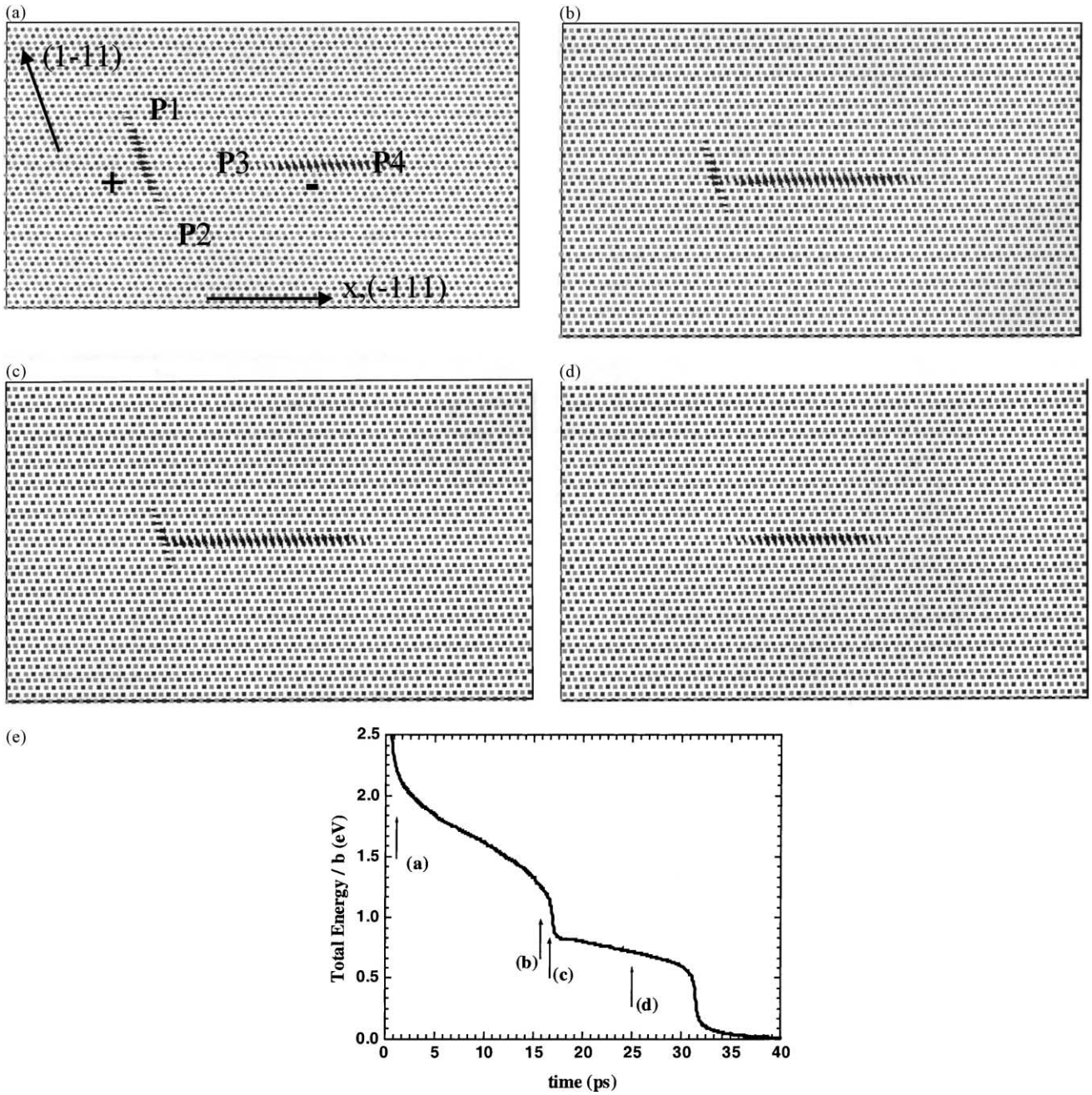

Fig. 2. Dislocation dipole annihilation. Differential displacement maps at different times (ps): (a) $t = 0$; (b) $t = 16$; (c) $t = 1.75$, and (d) $t = 25$. (e) Shows the time evolution of the total energy of the system.

associated with the snapshots in Fig. 2a–d. When annihilation between partials happens (at times ~17 and ~27 ps), the total energy of the system dramatically decreases by ~0.5 eV/b; this is the energy of two partials, see Section 3.1.

3.3. Dislocation dipole annihilation: dissociation on parallel planes

An interesting parameter, related to cross-slip, is the minimum stable dipole distance of opposite signed screw dislocations dissociated on parallel planes, see Fig. 3a. In this configuration, both dislocations need to cross-slip in order to annihilate. We study the structure and core energy of this configuration as a function of distance between the dissociation planes D_o.

In order to cross-slip, the two partials need to approach each other on their primary slip plane; when the distance between the partials (D_e) is less than a critical distance they can cross-slip. Both D_e and the core energy depend on D_o. In Fig. 3b, we plotted D_e and E_c as a function of D_o. As

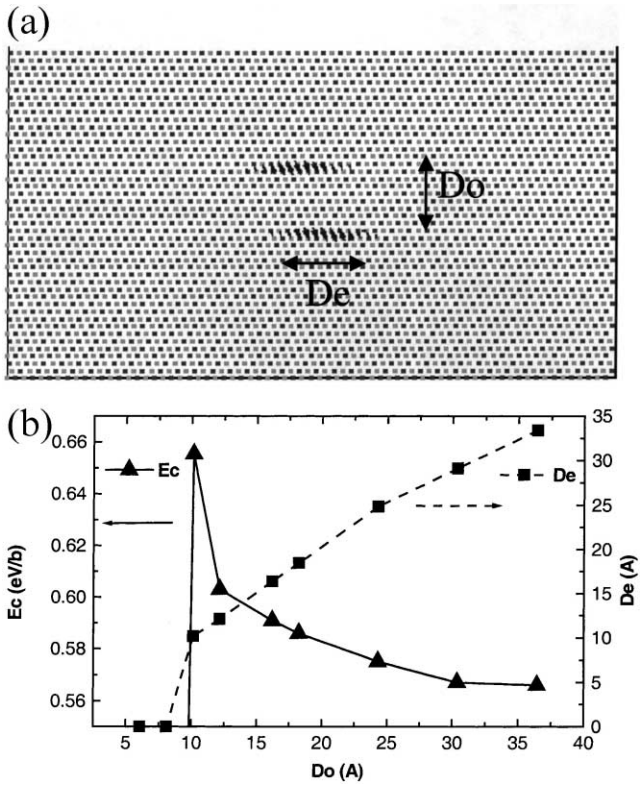

Fig. 3. Dislocation dipole dissociated on parallel planes: (a) differential displacement map of the system set-up; (b) core energy (left vertical axis) and separation between partials (right vertical axis) as a function of the distance between the planes.

expected, D_e decreases and E_c increases as the dislocations get closer. When the dipole separation D_o is <8 Å, the dislocations cross-slip and annihilate. We obtain the energy barrier for this cross-slip process to be 0.1 eV/*b*.

4. Conclusions

We studied the $1/2a\langle 1\,1\,0\rangle$ screw dislocation in Ni, which dissociates into two partials separated by 25 Å; the core energy is 0.5 eV/*b*. Using molecular dynamics (MD), we studied dislocation motion and annihilation.

The annihilation process of a screw dipole depends on how the two dissociation planes are configured. When the two dislocations dissociate into intersecting planes, we find that one dislocation cross-slips in the presence of a third partial coming from the opposite signed dislocation.

We also studied two opposite signed dislocations dissociated in parallel planes as a function of the distance between the planes. We find that the separation between the partials diminishes and the core energy increases as the two dissociation planes become closer. When the dipole separation is 8 Å, the dislocations cross-slip and annihilate. We calculate the activation energy for this cross-slip process to be 0.1 eV/*b*.

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