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Atomistic Simulation of kinks for 1/2a<111> Screw Dislocation in Ta

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ABSTRACT

We study the structure and formation energy of kinks in 1/2a<111> screw dislocation in metallic Ta Embedded Atom Model Force Field parameterized using quantum mechanical computations. We studied a/3<112> kinks using a simulation cell containing four dislocations in a quadrupole arrangement. We impose periodic boundary conditions in the directions perpendicular to [111] and fixed boundaries in the [111] direction. We find that two, energetically equivalent, core configurations for the 1/2a<111> dislocation lead to 8 distinguishable single kinks and 16 kink pairs. The different mismatches of core configurations along [111] direction cause variations in kink formation energy. The lowest formation energy of a kink pair is determined to be 0.73 eV. The geometric features of such kink pair have been studied with the help of structural analysis of the atomistic model. We also compare the activation energy for dislocation motion via the double kink mechanism with the activation energy for a rigid dislocation motion from a dipole annihilation simulation. We find that the migration energy for dislocation motion via double kink formation is 0.016 eV/b, which is less than the quarter of the migration energy associated with the kink free motion of a straight dislocation, 0.073 eV/b.

INTRODUCTION

Dislocations, and their interactions with other defects, are responsible for the plastic deformation in materials. The studies on structural, energetic and dynamic properties of dislocations are of importance in the design and processing of materials, especially for metals. Although new experimental techniques, such as the scanning tunneling microscope (STM), high-resolution transmission electron microscope (HRTEM), etc., are able to observe the structure of the defects in crystals at atomistic level, most of the details on the structure and mobility of dislocations are currently beyond the reach of experiment. Hence, the atomistic level simulation becomes a reliable approach to unveil the secrets about dislocation. In bcc metals, the screw dislocations have lower mobility than the edge components. They have a prevalent role on the low temperature plastic deformation. Especially for this reason, the property and behavior of a/2<111> screw dislocation have been studied extensively by atomistic simulations. [1,2]

Dislocations structure and the mechanism by which they move at T=0 K are different from those at finite temperatures. At T=0 K, dislocations are straight linear defects. When they move, all atoms along the dislocation move in unison. While, at finite temperatures, dislocations are no longer perfect straight lines. Different segments of dislocation may be in different equilibrium positions on its potential energy surface. Kinks, the region connecting neighboring dislocation segments at different equilibrium positions, are considered as defects of dislocations and play an essential role in the dislocation slip. The motion of dislocations is a repeating process of kink pair nucleation and subsequent sideways motion of the kinks. In the development

of a mesoscale dislocation theory, the kink pair formation energy and the minimum separation for a stable kink pair are important parameters that play a central role in describing the plasticity of materials [3]. In this paper, we present atomistic simulation results on kink formation energy and geometric features of kinks as well as the dynamic process of kink pair formation during the dislocation motion in metallic tantalum.

SIMULATION MODELS

Model of dislocation with build-in kinks: The simulation cells used to simulate kinks are orthorhombic and oriented in three orthogonal crystal directions, namely **X**: [11-2], **Y**: [1-10] and **Z**: [111]. There are three distinct regions along the dislocation line (**Z**) in the model. The upper and lower regions contain four equilibrated a/2<111> screw dislocations arranged as quadrupole, in which there is a pair of dislocations with Burgers vector b=a/2[111] and the other pair of dislocations with b=a/2[-1-1-1]. The positions of the dislocations in the upper and lower region differ by a/3<112>, i.e. the distance separating the nearest neighboring equilibrium positions of dislocations. The central region smoothes the interface discontinuity between upper and lower region. Once the model cell containing the four kinks is built, we relax the atomic positions by minimizing the energy of the system. We impose periodic boundary conditions in the directions perpendicular to the dislocations and fixed boundary conditions along the dislocation; we fix the atomic positions of two 5b thick regions at both ends of the cell to the relaxed dislocation configuration. In this study, we used simulation cells with cell lengths of 5a[1-12], 9a[1-10] and 150a/2[111]. It contains 40500 atoms (37800 movable) and the volume is 40.7 x 42.3 x 431.8 $Å^3$. Neglecting the interactions between the kinks we calculate the kink formation energy as one fourth of the energy difference between the quadrupole for relaxed dislocation with kinks and the quadrupole for equilibrated straight dislocations with same length.

Model of dislocations with nucleated kinks: As already mentioned, we are interested not only in equilibrium properties of kinks but also in their dynamical properties such as nucleation of kink pairs and their propagation along the dislocation. The process of kink pair nucleation is hard to study atomistically because the relatively short dislocations (~ hundreds of Burgers vectors) and short times (~ hundreds of picoseconds) make the nucleation very unlikely to happen during the course of a MD simulation. To remedy this, we studied the process of migration and annihilation of a <110> oriented dipole of screw dislocations via MD at T=0.001 K and provide a nucleation center for the kink pair by introducing a vacancy in the path of a dislocation (denote as D_v). The other dislocation (D_f) sees a defect-free environment. We use a relatively long simulation cell containing N=56700 atoms and lengths of 9a[1-12]=73.356 Å, 15a[1-10]=70.548 Å and 70a/2[111] =201.5 Å. We find that dislocations and vacancies attract each other; for Ta we calculated the vacancy formation energy in the core of a screw dislocation to be 2.45 eV while the vacancy formation energy in the bulk is 2.95 eV.

RESULTS AND DISCUSSION

Dislocation core structure and its effect on kinks: In our study, we find that the equilibrium a/2<111> screw dislocation core spreads out along three <112> directions in {110} planes; this feature can be clearly seen in differential displacement maps [figure 1 (a) and (b)]. In the map,[4] the local strain between neighboring atoms is drawn as arrow. There are six equivalent and homogeneously distributed <112> directions perpendicular to the dislocation line in bcc lattice and this leads to two different, but energetically equivalent, core configurations. The concept of polarization of the dislocation core can be used to distinguish these two core configurations and is shown in figure 1 (c) and (d). In these plots, the relaxed displacement of each atom along [111] direction is compared with that corresponding to a dislocation constructed according to elastic theory. The displacement differences for atoms other than the 6 columns closest to the dislocation line are less than +/- 0.05Å while the three central 3 atoms translate simultaneously 0.267Å (~0.09b) either in [111] or [-1-1-1] direction after relaxation. A dislocation is named positive (P) if the three central atoms translate in the [111] [as shown in figure 1(c)] and negative (N) if they shift in the [-1-1-1] [as shown in figure 1(d)].

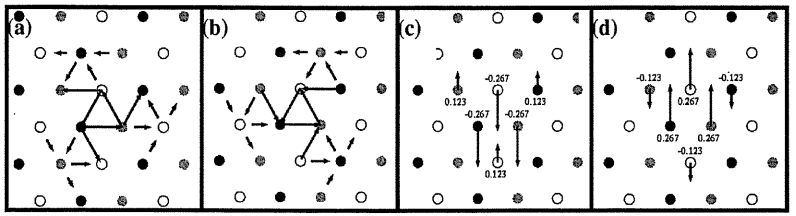

Figure 1. Equilibrated core of dislocation whose Burger vector is a/2[111]. In the figure, circles represent the (111) projection of atoms. Panel (a) and (b) are differential displacement maps showing two fashions of dislocation core spreading out along three <112> directions on {110} planes while panel (c) and (d) show the different polarization phenomena of the dislocation core shown in (a) and (b), respectively.

By geometry, there are two categories of kinks in a/2<111> screw dislocation in bcc Ta. We name a kink as right kink (R) when the kink vector is a/3[11-2] and left kink (L) when kink vector is -a/3[-1-12]. The kink vector is the vector from equilibrium dislocation position below the kink pointing to equilibrium dislocation position above the kink. The combination of the two core configurations (P and N) with the two directions (R and L) lead to eight single kinks (NRP, NRN, PRP, PRN, NLP, NLN, PLP and PLN). We have calculated the formation energies for all possibilities giving 0.62eV, 0.60eV, 0.60eV, 0.58eV, 1.12eV, 0.60eV, 0.60eV and 0.11eV, respectively. Among these kinks, NRN and PRP kinks are energy degenerate and related by symmetry operations, so are NLN and PLP kinks. The simplest kink pair is composed of a right kink and a left kink. In some cases, one or two flips are required to fulfill the requirement of core configurations to form a kink pair from a straight dislocation. The flip is the defect region where dislocation core changes to the other one in the dislocation line. There are P-N whose formation energy is 0.005eV and N-P whose formation energy is 0.57eV two types of flips. In P-N flip, the P type dislocation core changes to the N type dislocation core along [111] direction. The formation energy for a kink pair is defined as the summation of formation energies of its components (single kinks and flips). We find that the NRP-PLN kink pair has the lowest formation energy among 16 possible kink pairs and the formation energy is 0.73eV.

Structure analysis of NRP and PLN kinks: Besides the kink formation energy, geometric features are also essential in understanding plasticity in bcc metals. To determine these geometric parameters, we carried out a detailed structural and energetic analysis for the various kinks. We focus here on the single NRP and PLN kink that lead to the lowest energy kink pair and consequently the most important in order to determine the mobility of dislocations at low temperatures. In figure 2, the results on NRP and PLN kink are presented.

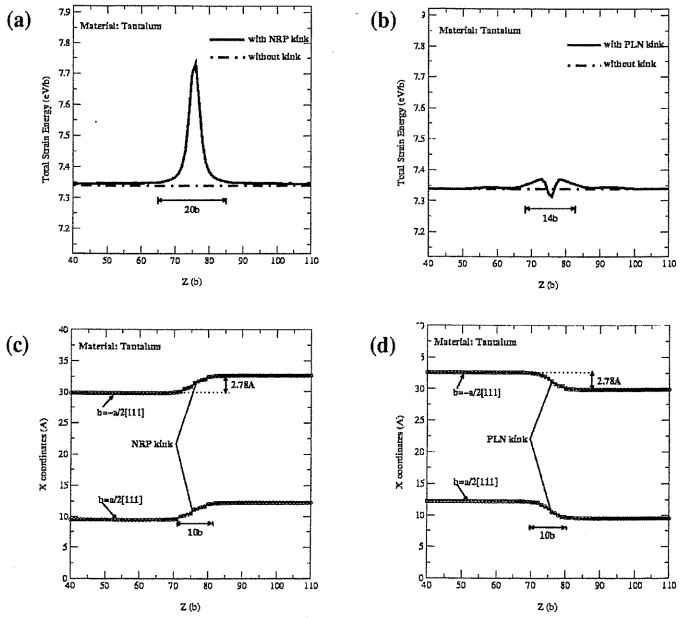

Figure 2. Panel (a) and (b) are plots showing strain energy distribution along dislocation of NRP and PLN kink, respectively. Panel (c) and (d) are plots showing dislocation core positions along dislocation line of NRP and PLN kink, respectively. In the plots, the system is divided into slices with thickness equal to Burgers vector b and strain energy or dislocation position is computed for each slice.

In figure 2 (a) and (b), the total strain energy distribution in [111] direction for a quadrupole of dislocations with NRP or PLN kinks and a quadrupole of straight dislocations are plotted. The strain energy is calculated as the summation of atomic stain energy, [the energy of each atom minus the cohesive energy in perfect bcc crystal] for all atoms in a slice with thickness b along the dislocation line. In figure 2 (c) and (d), we also plot the dislocation core position along the dislocation line for two of the dislocations in the quadrupole. The dislocation core position is determined as the atomistic strain energy weighted geometric center of 12 atoms closest to the dislocation line. From figure 2(c) and (d), we can determine the structure length for

NRP and PLN kinks to be 10b and structure height of these kinks to be 2.78A. The incipient length $L^{NRP-PLN}$, the minimal separation at which the NRP and PLN kinks would not annihilate to each other in a kink pair, can be estimated by combination of figure 2(a) and (b). From the point of view of energy, the distance between two undisturbed dislocation segments is 20 b for NRP kink and 14 b for PLN kink. Hence, $L^{NRP-PLN}$ could be evaluated to be 17b.

The process of kink pair formation and migration:

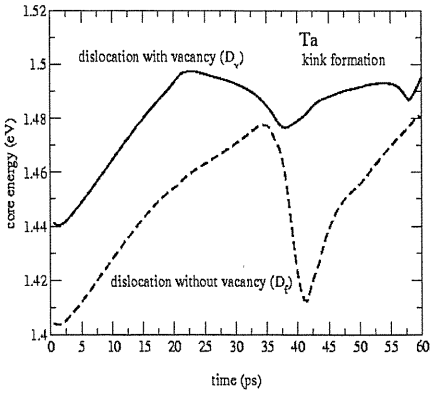

Figure 3: Core energy as a function of time for dislocation dipole annihilation. The full line corresponds to the dislocation with a vacancy in its path nucleating a kink pair to reduce the activation energy.

From our MD simulations of dipole annihilation we find that the vacancy helps nucleate a kink pair that propagates making the dislocation advance. In Figure 3 we show the core energy per Burgers vector as a function of time for two dislocations (D_v and D_f). The core energy is defined as the strain energy of the 12 atoms with higher energy per dislocation, per Burgers vector. The dislocation without the vacancy (D_f) shows the same motion behavior we found in smaller (7 b long) cells,[2] shown as the dashed line in the figure 3. It moves as a rigid straight line with an activation barrier of 0.07 eV/b. On the other hand, the dislocation with the vacancy in its way (D_v) moves faster and experiences a lower energy barrier. The activation energy for the first jump of D_v (0.6 eV/b) is very similar to the one corresponding to a rigid dislocation but after the maximum, the energy does not reach the initial relaxed value. As explained below, this is due to the presence of a kink pair.

In Figure 4(a), we show the position profile of dislocation D_v (z and y represent the position of the dislocation in [111] and [11-2] directions in the plot) from 20 to 37.5 ps. Figure 4(b) shows core energy along the dislocation line at the same times. We can see that at t = 20 ps the dislocation is almost perfectly straight and the core energy is constant along the dislocation line notice that the position of the dislocation and core energy are affected by the presence of the vacancy with a z position close to zero. At time t = 30 ps a kink pair can be clearly seen both from the dislocation profile and core energy (note that we have periodic boundary conditions). Part of the dislocation line has advanced to the next equilibrium position while the middle part of D_v (from z~60Å to z~125Å) is still climbing the Peierls potential barrier. From Figure 4 (b) we see that the core energy is lower for the portions of the dislocation that advanced and is still higher in the middle part of our simulation cell. The asymmetry in the energy plots comes from the fact that the kink pair contains two different kinks as explained in the previous subsection.

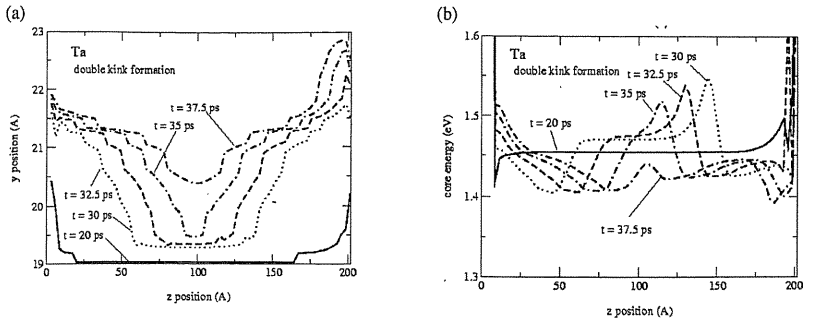

Figure 4. (a) Profile of dislocation D_y (y position of the dislocation along the dislocation line) at different times form 20 to 37.5 ps. (b) Core energy along the dislocation line for the same times.

CONCLUDING REMARKS

Kink pair nucleation followed by kink migration is the main mechanism determining the mobility of screw dislocations in bcc metals. The atomistic simulation provides a unique avenue to study the details of these processes and provides a link between atomic interactions and the mechanical properties of materials. We have used MD with a First Principles Force Field to study both equilibrium and dynamical properties of single kinks and kink pairs. We calculated the structure and energy of various single kinks as well as the dynamical process of kink pair nucleation and migration. The atomistic information is invaluable to validate and *inform* mesoscopic and continuum models of plasticity [5]. Such multi-scale approaches, based on *ab-initio* calculations will play an important role in the development of next-generation materials.

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