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Molecular dynamics simulations of 1/2 $a\langle 1\ 1\ 1\rangle$ screw dislocation in Ta

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Abstract

Using a new, first principles based, embedded-atom-method (EAM) potential for tantalum (Ta), we have carried out molecular dynamics (MD) simulations to investigate the core structure, core energy and Peierls energy barrier and stress for the 1/2 $a\langle 1\ 1\ 1\rangle$ screw dislocation. Equilibrated core structures were obtained by relaxation of dislocation quadrupoles with periodic boundary conditions. We found that the equilibrium dislocation core has three-fold symmetry and spreads out in three $\langle 1\ 1\ 2\rangle$ directions on $\{1\ 1\ 0\}$ planes. Core energy per Burgers vector b was determined to be 1.36 eV/b. We studied dislocation motion and annihilation via molecular dynamics simulations of a periodic dislocation dipole cell, with $\langle 1\ 1\ 2\rangle$ and $\langle 1\ 1\ 0\rangle$ dipole orientation. In both cases the dislocations move in zigzag on primary $\{1\ 1\ 0\}$ planes. Atoms forming the dislocation cores are distinguished based on their atomic energy. In this way, we can accurately define the core energy and its position not only for equilibrium configurations but also during dislocation motion. Peierls energy barrier was computed to be $\sim$0.07 eV/b with a Peierls stress of $\sim 0.03\mu$, where μ is the bulk shear modulus of perfect crystal. The preferred slipping system at low temperature is $\langle 1\ 1\ 2\rangle$ directions and $\{1\ 1\ 0\}$ planes.

Keywords: Dislocation; Molecular dynamics; Tantalum

1. Introduction

Low temperature plasticity in bcc metals is governed by the 1/2$a\langle 1\ 1\ 1\rangle$ screw dislocations due to their low mobility as compared to edge segments. Thus, the theoretical understanding of their properties is of great importance [1–3].

With the fast development of powerful computers, atomistic simulations using chemically and physically realistic models are becoming quite important in characterizing the structure and properties of materials. 1/2 $a\langle 1\ 1\ 1\rangle$ screw dislocations in bcc metals have been studied using different simulation techniques. Moriarty and coworkers investigated the core structure, core energy, Peierls stress and kink-pair formation energy for 1/2 $a\langle 1\ 1\ 1\rangle$ screw dislocation in molybdenum and tantalum, using multi-ion interatomic potentials for transition metals from first principles generalized pseudopotential theory (MGPT) [4,5]. Recently, Ismail-Beigi and Arias studied the 1/2a $\langle 1\ 1\ 1\rangle$ screw dislocation in Mo and Ta with ab initio (DFT-LDA) method [6].

In this paper, we present atomistic simulations of core structure and energy, dislocation annihilation, Peierls energy barrier and stress for 1/2$a\langle 1\ 1\ 1\rangle$ screw dislocation in tantalum (Ta). We use a new, first principles based, embedded atom model force field (named qEAM FF) for Ta [7]. The functional form of the qEAM FF is based on [8] and we will only mention the differences. We added volume dependence to the electronic density; the parameter α in Eq. 32 in Ref. [8] is replaced by $\alpha/V^{1/3}$, where V is the volume per atom. We also included one more term ($f_4 a^{*4}$) in the embedding energy, Eq. 33b in Ref. [8]. The parameters for the qEAM FF for Ta are (the units for b_i are eV/Å$^{(4+i)}$): Å r_m(Å) = 4.81253968; b_0 = 6.50281587; b_1 = −11.26455130; b_2 = 8.01451544; b_3 = −2.97299223; b_4 = 0.60004206; b_5 = −0.06222106; b_6 = 0.00258801; b_7 = −0.00000504; a_1 = 0.07293238; a_2 = 0.15781672; α(1/Å) = 21.79609053; β = 7.79329426; a_0(Å) = 3.32389219; E_{coh}(eV) = 8.154204; B_T(Mbar) = 1.830354; λ = 0.207828; k = −0.00717801; f_4 = −0.00000504.

In Section 2, we present our results on core structure and energy using a quadrupolar dislocation system. In Section 3, we study motion and annihilation of opposite signed dislocation. From this process, we calculate the Peierls energy barrier and stress. Finally, in Section 4 conclusions are drawn.

2. 1/2a $\langle 1\ 1\ 1\rangle$ screw dislocation core energy and structure

In order to investigate the core energy and structure of 1/2$a\langle 1\ 1\ 1\rangle$ screw dislocation in Ta, we build a dislocation quadrupole in our simulation cell and impose periodic boundary conditions. Two dislocations have Burgers vector $b = 1/2a\langle 1\ 1\ 1\rangle$ and the other two $b = 1/2a\langle$-1-1-1$\rangle$. Such

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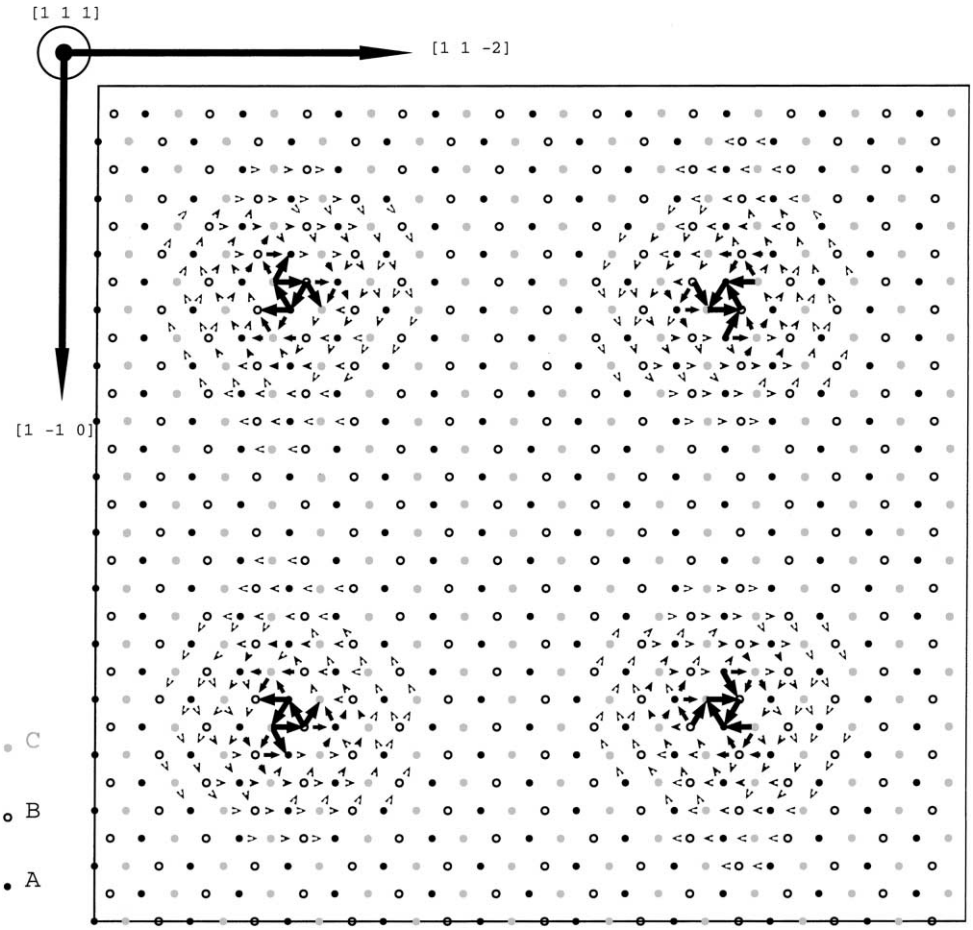

Fig. 1. Differential displacement map (DDM) of equilibrated dislocation quadrupole.

arrangement of dislocations minimizes the misfit of atoms on the periodic boundary due to the effects of periodic images. The initial dislocations are constructed according to elastic theory and then we relax the atomic coordinates using the qEAM FF. In the bcc structure, there are two kinds of dislocation core configurations (easy core and hard core) that can be transformed to each other by reversing the Burgers vector. In this work we focus on the lower energy easy cores. In Fig. 1 we show the differential displacement map (DDM) of the relaxed quadrupole system. In the DDM atoms are represented by circles and projected on a (1 1 1) plane. The arrows represent the relative displacement in [1 1 1] direction of neighboring atoms due to the dislocation. We can see from Fig. 1 that the equilibrium dislocation core obtained using qEAM FF has three-fold symmetry and spreads out in three $\langle 1\,1\,2\rangle$ directions on $\{1\,1\,0\}$ planes.

We define strain energy as the total energy of our system once the perfect crystal energy is subtracted. The total strain energy can be divided in two terms: core energy (E_c) and elastic energy (E_e). The latter contains the self-energy of each dislocation and their interactions and can be calculated using linear elasticity theory. The core energy is the energy contained close to the dislocation line (closer than some distance r_c called core radius) where, due to the large strain, elasticity theory is not valid and the details of the interatomic interactions are important. For our quadrupole system the total strain energy takes the form [6]

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

where K depends on the elastic constants, d_1 and d_2 are the nearest separation of dislocations along $\langle 1\,1\text{-}2\rangle$ and $\langle 1\text{-}1\,0\rangle$ directions and $A(d_1/d_2)$ is a geometric factor which comes from the dislocation interactions.

We studied quadrupolar dislocation cells of different sizes. In Fig. 2 we show the minimized energy as a function of $\ln(d_1/r_c) + A(d_1/d_2)$ for the different simulation cells; in order to compare with previous calculations [4–6] we took $r_c = 2b$. We can see that the total energies follow a straight line as predicted by elasticity theory (Eq. (1)), showing that the value chosen for the core radius $r_c = 2b$ is large enough to take account for the non-elastic region near the dislocation line. From a linear fit to our data we determine the core energy $E_c = 1.36\,\text{eV}/b$ and $K = 2.77 \times 10^{-2}\,\text{eV}/A^3$. The value of K can also be computed from the elastic constants giving $2.97 \times 10^{-2}\,\text{eV}/A^3$ very similar to the one obtained

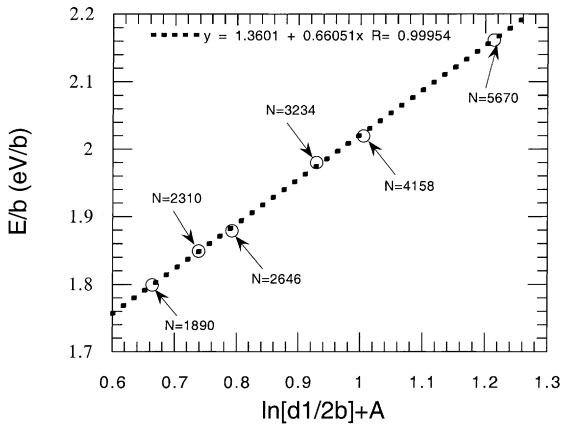

Fig. 2. Plot of E/b vs. $\ln[d_1/2b] + A(d_1/d_2)$. The dotted line represents the linear fit, $E/b = 1.3601 + 0.6605\ [\ln(d_1/2b) + A(d_1/d_2)]$. The total number of atoms in each simulation cell is shown.

from the fit. Recent ab initio calculations of core energy give 0.86 eV/b, lower than the value obtained with qEAM FF and the dislocation cores are compact and symmetric [6] (Fig. 2).

Using the qEAM we can calculate the strain energy associated with each atom. In Fig. 3 we show the atomic energy distribution (number of atoms per dislocation per Burgers vector as a function of their strain energy) for a system containing 5670 atoms in the periodic cell. We can see that there are six atoms with atomic strain energy higher than 0.15 eV and another six atoms with energy in the range 0.06–0.08 eV. They correspond to the 12 atoms per dislocation per Burgers vector closer to the dislocation line and their total energy is ∼1.4 eV/b, very similar to the core energy obtained from Eq. (1). The rest of the atoms have low strain energy and make the elastic part of the system. We can then define the dislocation core as the 12 atoms per Burgers vector with higher energy.

3. Dislocation motion: dipole annihilation

In order to study dislocation motion we build a dislocation dipole along a ⟨1 1 0⟩ direction in our simulation cell with periodic boundary conditions. We then perform a TVN MD simulation at a very low temperature ($T = 0.001$ K). Due to the attractive interaction between dislocations with opposite Burgers vectors the two dislocations forming the dipole move towards each other and eventually annihilate. The dislocations move in a zigzag style and the slip system is ⟨1 1 2⟩ directions on {1 1 0} planes.

The solid line in Fig. 4 shows the time evolution of the total strain energy per dislocation per Burgers vector from our MD simulation. We can see that the strain energy decreases as the dislocations approach each other. It is also clear the presence of small "energy bumps" during the dislocation motion; these bumps are due to the Peierls energy landscape that the cores have to overcome in order to move. Finally, the process of annihilation can be identified in Fig. 4 by a rapid decrease of strain energy at time $t \approx 125$ ps; the distance between the dislocations when annihilation happens is ∼8 Å. Once the dislocations annihilate we have a perfect bcc crystal and the strain energy is zero.

We can separate the total strain energy in Fig. 4 into core and elastic parts using the core definition proposed in the last paragraph of last section: the core is composed of the 12 atoms per dislocation per Burgers vector with higher energy. In Fig. 4 we also show the time evolution of the core energy (dashed line) and elastic energy (dotted line). We can see that the core energy shows a periodic behavior and that the elastic energy decreases monotonically and does not exhibit the "energy bumps" present in the total energy.

Peierls stress (also called critical resolved shear stress (τ_{CRSS})) rather than Peierls potential barrier can be measured experimentally. When shear stress resolved on the slip plane and in the slip direction reaches τ_{CRSS} the dislocation

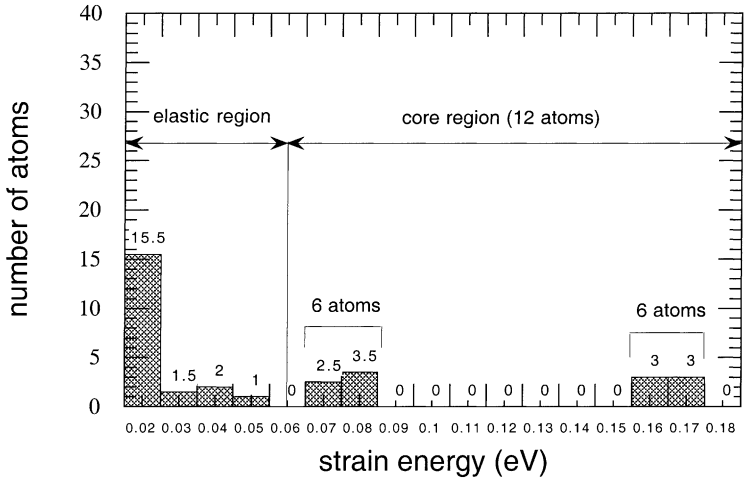

Fig. 3. Histogram of atomistic strain energy distribution for quadrupolar arrangement of dislocations. The cell contains 5670 atoms and dislocations are 7 Burgers vectors long.

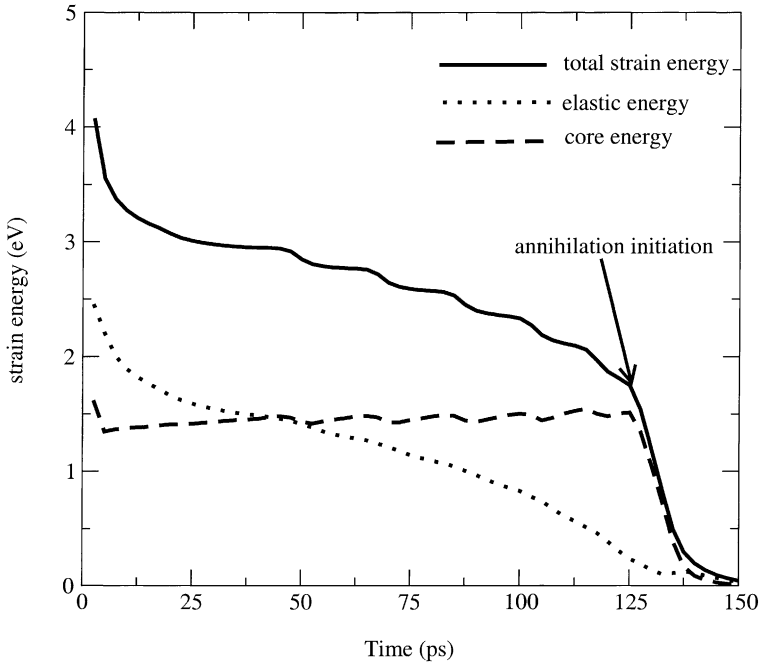

Fig. 4. Strain energy (solid line), elastic energy (dotted line) and core energy (dashed line) as a function of time during the dislocation dipole migration and annihilation.

starts to move. τ_{CRSS} is defined by [9]

$$\tau_{\mathrm{CRSS}} = \mathrm{MAX}\left[\frac{1}{b}\frac{\mathrm{d}W(x)}{\mathrm{d}x}\right]$$

where b is the Burgers vector, $W(x)$ is the core energy per b when the dislocation moved a distance x on the slip plane and in the slip direction.

In order to compute the stress [$\tau = 1/b\mathrm{d}W(x)/\mathrm{d}x$], we need to calculate the dislocation core position at any time during its motion. We define the dislocation position as the geometric mean position of the core atoms weighted with their atomic strain energy. Fig. 5(a) shows the dislocation core energy as a function of the distance travelled by the dislocation. We can see that the dislocation core energy varies periodically with a period of 2.72Å = $|1/3a\langle 112\rangle|$, the Peierls energy barrier is ~0.07 eV/b. In Fig. 5(b) we show the stress as a function of the distance travelled by the dislocation. The Peierls stress obtained from our simulations is ~1.8 GPa or ~0.031μ where μ is the shear modulus. Defining the core as the 9 or 15 atoms with higher energy per dislocation per Burgers vector gives a Peierls energy of 0.071 and 0.073 eV, respectively, very similar to the ones obtained

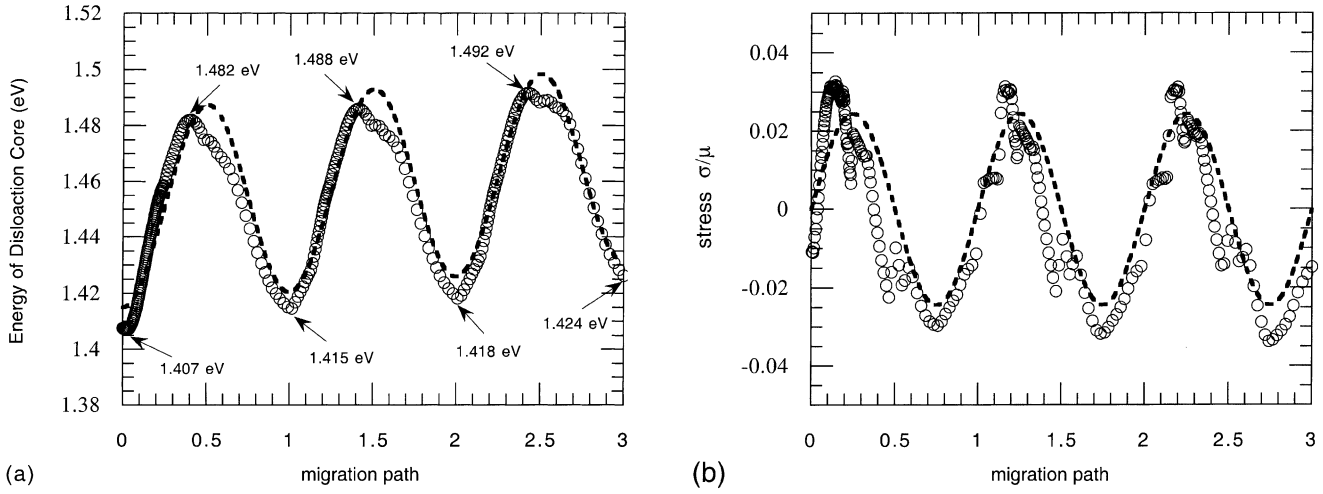

Fig. 5. (a) Dislocation core energy as a function of distance travelled by the dislocation. The dotted line represents a cosine fit to the data; (b) stress as a function of distance. The unit of migration path is $|1/3a\langle 1\,1\,2\rangle|$.

using 12 atoms. Similar value for the Peierls stress (0.022μ) was obtained by Moriarty et al. using MGPT potential [5].

4. Discussion

Using a new many body force field with molecular dynamics we investigate, from an atomistic point of view, static and dynamical properties of $1/2a\langle 1\,1\,1\rangle$ screw dislocations in Ta. Using a dislocation quadrupole and elasticity theory we calculate the core energy (1.36 eV/b). We find the dislocation cores to be asymmetric and spread in three $\langle 1\,1\,2\rangle$ directions; on the contrary recent ab initio results show symmetric and compact cores [6].

By studying the strain energy associated with each atom we can define the core as formed by the 12 atoms per Burgers vector with higher energy. Using this definition of core to analyze the motion of a dislocation dipole configuration we can obtain the Peierls energy barrier (0.07 eV/b) and Peierls stress ($\sim 0.031\mu$).

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