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Dislocation motion in BCC metals by molecular dynamics

Jinpeng Chang [a,*], Wei Cai [a], Vasily V. Bulatov [b], Sidney Yip [a]

[a] *Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*
[b] *L-369, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA*

Abstract

We performed molecular dynamics (MD) simulation of edge dislocations in BCC metal Mo with 1/2⟨1 1 1⟩ Burgers vector gliding on (1 1 0) plane using the Finnis–Sinclair N-body empirical potential and periodic boundary conditions (PBC). The profile of dislocation line, extracted from atomic displacements during MD simulation, suggests a dominant mechanism of double-kink nucleation, without appreciable kink migration. This observation is consistent with further simulations in which dislocations with pre-existing kinks are observed to move at the same velocity as the initially straight dislocations. Our results show a linear stress dependence of the dislocation velocity and a decrease of mobility with increasing temperature, both features interpreted as signifying that the simulations pertain to the viscous phonon drag regime of dislocation mobility.

Keywords: Dislocation mobility; Molecular dynamics; Molybdenum

1. Introduction

Studying dislocation motion in BCC metals by direct molecular dynamics (MD) simulations is important both for providing quantitative predictions of dislocation mobility, and for understanding the underlying atomistic mechanisms governing the complex plastic deformation behavior in BCC metals [1,2]. Such simulations have proved to be difficult heretofore, largely because of the limited time scale of MD simulations (usually in picoseconds) and the complexity of setting up appropriate dislocation microstructure for systems with limited number of particles. In this work, we demonstrate the feasibility of direct MD study of edge dislocation motion, since edge dislocations are much easier to move than screw dislocations in BCC metals. By employing a periodic boundary condition (PBC) with constant applied shear stress, steady state dislocation motion is achieved in the simulation, thus enabling a quantitative prediction of dislocation velocity. The potential model we use for the MD simulation is a Finnis–Sinclair potential model modified by Ackland and Thetford [3,4]. In Section 2, we present the methods of setting up the simulation cell and extracting dislocation positions during the simulation. In Section 3, we discuss the results on the mechanism of dislocation motion and the temperature and stress dependence of dislocation velocity.

2. Simulation methods

2.1. System setup

As shown in Fig. 1, the simulation cell is initially a rectangular box of atoms with periodic boundary conditions (PBC) where the three repeat directions are along [1 1 1], [$\bar{1}$ 0 1] and [1 $\bar{2}$ 1]. A dislocation dipole is created by removing a layer of atoms on the shaded plane in Fig. 1, displacing the neighboring atoms according to linear elastic displacement fields, and relaxing the entire structure using the conjugate gradient method. The dislocations thus created have a Burgers vector 1/2[1 1 1] and will move on the glide plane ($\bar{1}$ 0 1). During the simulation, the two dislocations move on their own glide planes, which are separated by half of the simulation box height. This height is chosen to be as large as possible to minimize the interactions between the two dislocations.

This atomic configuration of straight dislocation dipole can be used to prepare configurations with kinked dislocations by placing another copy of the configuration from Fig. 1 behind the original one but with a slight offset of a/2[1 1 1] as shown in Fig. 2.

We apply a shear stress to the simulation cell using Parrinello–Rahman method [5] and constant system temperature is maintained by a soft velocity scaler.

2.2. Dynamic dislocation profile

During the simulation we analyze the particle coordinates to determine the dislocation core position for every

* Corresponding author.
E-mail address: jpchang@mit.edu (J. Chang).

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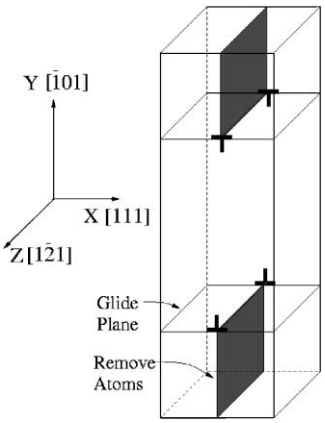

Fig. 1. Edge dislocation dipole created by removing the atoms in the shaded area followed by conjugate gradient relaxation.

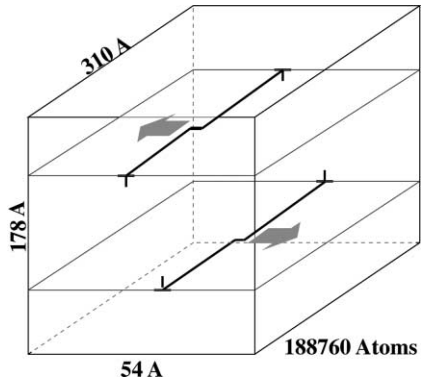

Fig. 2. Preparation of edge dislocations with single kink.

dislocation segment. We divide the simulation cell along the *Z*-axis into slices each of which contains only one dislocation segment and for each slice we only look at the two rows of atoms immediately above and below the slip plane. We calculate the disregistry between these two rows as a function of *X*-coordinate and then perform local parabolic fitting to find the location of maximum disregistry which we will regard as the dislocation core position for this segment.

Thus, we construct the profile of the dislocation line, and by repeating the procedure at successive timesteps we can follow the time evolution of the dislocation profile. The 3D plot in Fig. 3 shows how the dislocation line shape evolves with time. The dislocation line is 36 repeat distances long. As can be seen in the figure, the upward motion of the dislocation is accomplished by frequent nucleation of double kinks but few kink migration.

In the case of edge dislocation with an initial kink, we observed that the dislocation velocity is not affected by the pre-existence of the kink. This observation is consistent with that discussed in the previous paragraph and suggests that kink nucleation energy is much lower than kink migration energy for an edge dislocation. However, further MD and ab initio calculations have to be performed to confirm this interpretation.

By averaging the core position along the dislocation line we get the average line position of dislocation. Plotting it against time and fitting to a straight line, we extract the dislocation velocity as the slope of the fitted line.

3. Dislocation velocity

From a series of MD simulations we obtain an array of dislocation velocity data for temperatures ranging from 20 to 1000 K and shear stresses from 50 MPa to 5 GPa.

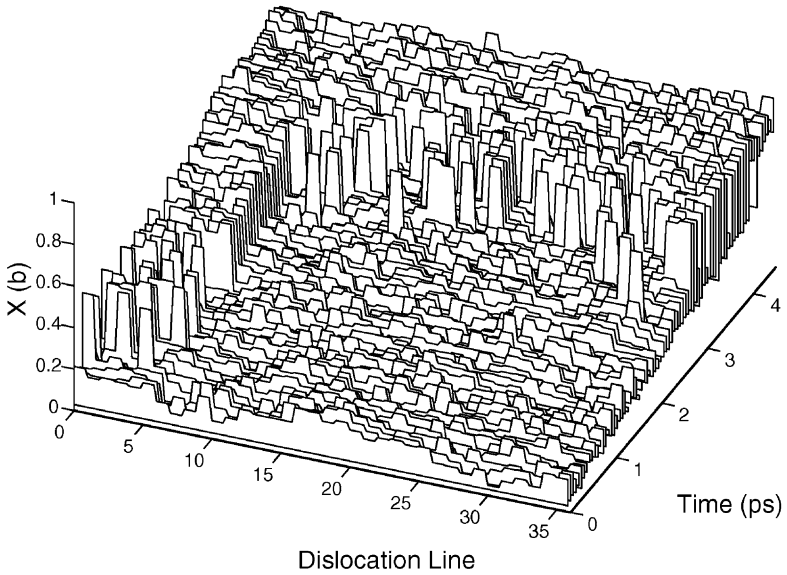

Fig. 3. Evolution of dislocation profile ($T = 20$ K, $\tau = 0.07$ GPa). Dislocation moves upward by frequent nucleation of double kinks of $b/3$ height.

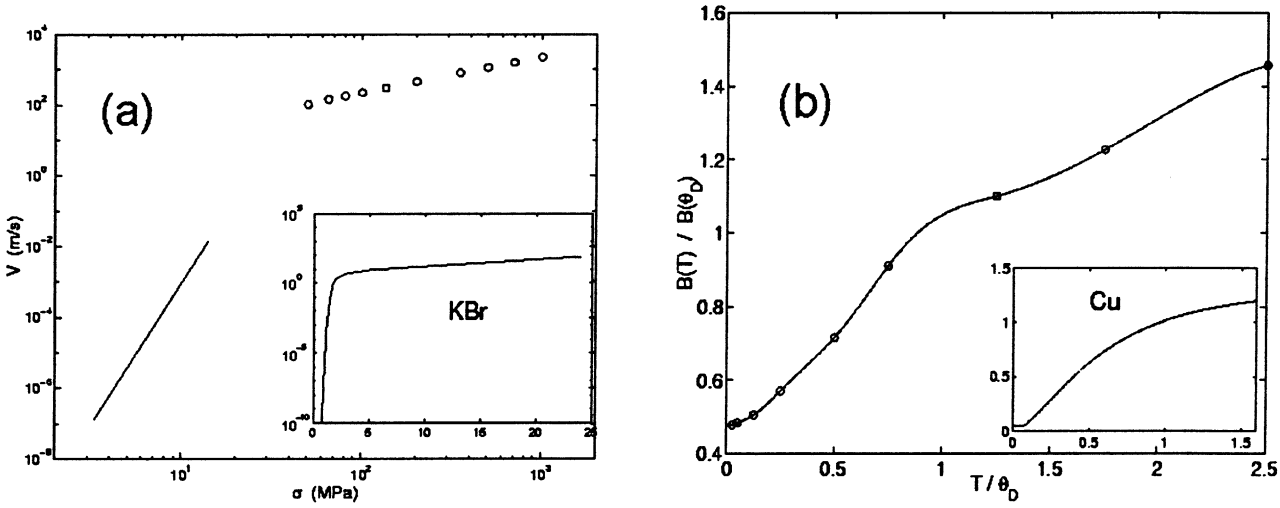

Fig. 4. (a) Stress dependence of velocity at T=77 K. MD results are plotted in open circles and experimental results [6] in solid line. The inset plots dislocation velocities (edge and screw) as a function of shear stress in calcium-doped KBr at room temperature where the stress exponent decreases from $m = 40$ to $m = 1$ [7]; (b) Temperature dependence of drag coefficient for edge dislocation. Normalized drag coefficient plotted against normalized temperature. (Debye temperature $\theta_D = 400$ K for Mo; $B(\theta_D) = 2 \times 10^{-4}$ Pa s). MD results are plotted in open circles and the inset figure plots experimental results for copper [8].

3.1. Stress dependence

It is conventional to represent dislocation velocity data by an empirical expression of the form $v \sim \tau^m \exp(-Q/kT)$ where m is the stress exponent. Fig. 4(a) shows that in the stress range we have studied, the stress exponent m is close to unity. The linear dependence of $v(\tau)$ is a distinctive feature of the high velocity region where drag mechanisms dominate. An obvious difference between the simulation and experimental results can be seen, the latter showing an exponent value close to 8. This may not be all that surprising because the MD simulations, given their microscopic nature and computational limitations, can only probe thus far the high-velocity, high-stress region. In contrast, experimental data are available only in the low-velocity, low-stress region. It may be possible to reach stresses comparable to the experimental range by resorting to acceleration techniques. This, however, remains to be demonstrated.. That a connection could exist between the high- and low-stress regions (and correspondingly high- and low-velocities) is indicated by the inset in Fig. 4(a) which shows experimental data for KBr displaying the characteristic behavior of both regions. We regard this as a reasonable basis for the expectation that the existing data on Mo and our simulation results may well be compatible with each other.

3.2. Temperature dependence

Another way to discuss the dislocation velocity data is through the drag coefficient defined as $B = b\tau/v$. One can see from Fig. 4(b) that the drag coefficient increases with increasing temperature. This is fundamentally different from the behavior in the thermal activated region where an Arrhenius relation holds. In the present high-velocity region, phonon drag is the governing mechanism [9]. Although there are no experimental data on the temperature dependence of the drag coefficient for Mo, experiments on other materials have shown a temperature variation very similar to our results, as indicated by the inset in Fig. 4(b). Theoretical calculations yield similar results [10].

4. Summary

We have simulated edge dislocation gliding on (1 1 0) plane in BCC metal molybdenum by direct molecular dynamics method using Finnis–Sinclair potential model. The dislocation line profile is extracted from atomic position data during the MD simulation leading to the observation that dislocation motion occurs by frequent double kink nucleation relative to kink migration. This suggests that kink nucleation energy barrier could be lower than that for kink migration. All our simulations are in the high-stress, high-velocity regime where phonon drag appears to be the dominant mechanism: in particular, the simulation data show a linear stress dependence of dislocation velocity and a decreasing velocity with increasing temperature, both features having been observed in experimental measurements on other materials.

In order to simulate low-stress, low-velocity region where dislocation motion is thermally activated, it would be necessary to implement hyperdynamics method [11,12] to extend the time scale of MD simulation. Additionally, meso scale modeling methods such as kinetic Monte Carlo also can be used [13,14] to overcome the size limitation of MD. Work

is currently underway to link atomistic and mesoscopic simulations for the ultimate goal of predictive modeling of dislocation microstructures and mechanical behavior.

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