Simulation of dislocation-phonon interaction in metals

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Abstract. Motion of dislocations interacting with phonons has been simulated by means of molecular dynamics method. The embedded atom method potential for copper is adopted in the simulation. Model crystal is a rectangular solid containing about 140000 atoms. An edge dislocation is introduced along [112] direction near centre of model crystal, and the system is relaxed. After the dislocation configuration is stabilized, a shear stress is applied and released. Wavy motions of dislocations developed on the Peierls valleys are observed. Excitation of atoms consisting the dislocation by the propagation of ‘hot atoms’ is also observed in the simulation.

1. Introduction
The mechanical relaxation due to dislocation has been observed in copper, aluminum and other metals by means of internal friction measurements. Broad relaxation peaks observed at temperatures between 100 K and 200 K in the deformed samples are called Bordoni peak. If these relaxation peaks are analyzed based on the double kink formation mechanism, a larger value of Peierls stress, $10^{-3} \mu$, is derived, where $\mu$ is the shear modulus [1]. One of the present authors Kosugi discovered a new relaxation peak at 11 K in zone refined aluminum samples, and derived Peierls stress was orders of $10^{-5}\mu$, which is reasonable size as expected from the plastic deformation experiments[2]. Such a low temperature peak is not observed in impure samples and in other metals. On the other hand, we have performed a molecular dynamics computer simulation of dislocation motion in 2-dimentional model. In the simulation, the total kinetic energy is found to make a bump in the time variation, when the dislocation surmount a Peierls potential hill. The Peierls stress is estimated to be the order of $10^{-3}\mu$ from the size of the bump[3]. The purpose of the present study is to develop a 3-dimentional model for the simulation of dislocation in copper, and investigate the static structure, dynamic properties of dislocation and interaction with phonons. A newly developed embedded atom method potential [4] was used in the present simulation. The potential function has successfully applied on the simulation of the dynamics of crystal defects and nanoparticles [5-7]

2. Method of simulation
Molecular dynamics simulation has been performed by using an EAM potential. Potential functions are developed by the present authors. The potential energy for $i$-th atom is expressed as

$$E_i = F(p_i) + (1/2) \sum \phi(r_{ij})$$

(1)
where $F(\rho_i)$ is the embedding energy for $i$-th atom, and $\rho_i$ is the electron density function. The Potential parameters for Cu are determined to reproduce the material properties such as the cohesive energy, the elastic constants, the vacancy formation energy and the stacking fault energy[4].

By using the potential function molecular dynamics simulation is performed, where the equation of motion is integrated numerically. The time interval $\Delta t$ for the simulation is chosen to be $1 \times 10^{-15}$ s, which is about 1/100 of the period of the maximum atomic vibrational frequency. Model crystal is surrounded by \{110\}, \{111\} and \{112\} faces, and consisted of 143000 atoms. Sizes are about 12x10x12 nm in $x$, $y$, $z$ directions, respectively. Mixed boundary conditions are adopted, namely, atoms on the surfaces parallel to the dislocation line are fixed and atoms on the surfaces perpendicular to the dislocation line are moved freely during simulation. Initially extra \{110\} planes are inserted in the lower middle of the crystal, and then the crystal is relaxed. The introduced dislocation is split to two partials as expected. One of the convenient ways to express the position and the structure of dislocation is investigated by highlighting the atoms, which have larger potential energy.

Configuration of atoms after initial relaxation is shown in figure 1. The potential energy of each atom is calculated by equation (1), and atoms with the potential energy larger than -3.2 eV are represented by solid circles. The solid circles are concentrated at the dislocation cores, and introduced dislocation is seen to be split to partials. The atoms shown by solid circles are seen to be spread in one of the \{111\} atomic plane, which is marked by ‘S’ in figure 1 (a). Vertical view of atomic planes surrounded by two straight lines in figure 1 (a) are shown in figure 1 (b). A stacking fault structure (hcp) is seen between two partial dislocations. Width of the stacking fault is determined as a balance of the stacking fault energy and the repulsive force between two partial dislocations, but the mirror force of fixed boundary may reduce the width of the stacking fault.

![Figure 1](image_url)

*Figure 1.* Configuration of atoms around the split edge dislocations after the initial relaxation. (a) perpendicular, and (b) parallel to the dislocation lines.
3. Results and Discussion

3.1. Motion of dislocation under a shear stress

A shear strain $\varepsilon_{xy} = 0.05$ to move the dislocations in -$x$ direction was applied, and system was relaxed. Then the motion of dislocations was monitored. The simulation was performed at the temperature, 0 K, but it was slightly increased up to 5 K with the time steps. Snap shots of the dislocation configuration at typical MD time steps are shown in figure 2, where only atoms with higher potential energy, $E > -3.5$ eV, are shown, and the atoms with the potential energy higher than -3.485 eV are shown by solid circles. These open and solid circles characterize the internal structure of the dislocations. The dislocations are very wavy and many kinks seem to be present on the Peierls hills, which run in vertical direction on a slip plane. The configurations shown in figure 2 are not symmetrical in $z$ direction. It is noted that six distinct types of atomic planes are stacked upon one another in a repeating sequence as ABCDEFABCDEF. in [112] direction, and it is not symmetric in a top and bottom direction. Initially the partial dislocation of left moved towards left by the applied stress, afterwards it was pushed back by the mirror force due to the fixed boundary. These motions were repeated. A period of the dislocation oscillation is about 10 ps, which is about 100 times of the period of thermal lattice vibration. As the dislocations are widely spread on a \{111\} plane $S$, shown in figure1 (a), and they are always confined in one of the atomic plane, namely, the clime motion is not observed in the present simulation.

Figure 2. Motion of split dislocations after applying a shear stress at (a) 0, (b) 1000, (c) 2000, (d) 3000, (e) 4000 and (f) 5000 molecular dynamics time steps.
Figure 3. Distribution of ‘hot atoms’ (a) at 100 MD steps, (b) at 150 MD steps and (c) at 200 MD steps in perfect crystal. (a’),(b’) and (c’) show the results in the crystal with dislocation.

3.2. Phonon absorption by dislocation
An initial velocity in y-direction is given to the atoms near the center of x-z plane, and the magnitude of the velocity of all atoms is monitored. An atom, which has larger magnitude of velocity than the criterion, is called ‘hot atom’. The simulation was performed in two samples of same size. One is the perfect crystal, and the other contains a split dislocation. Distribution of hot atom at typical time step of molecular dynamics in both sample are compared in figure 3, in which the hot atoms are marked by solid circles. Initially hot atoms are generated between two partials. A region occupied by hot atom is growing. When the border of hot atoms reaches the position of the split dislocations, many atoms constituting the dislocations are exited and become hot atoms. Atoms on the dislocation line are unstable and mobile, and start to move by the excitations. The phenomenon may be described as the absorption of phonons by some localized dislocation modes, but quantitative discussion on the dislocation localized mode has not yet made. The molecular dynamics will provide useful information on the problem.

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