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Simulation of Dislocation Dynamics in FCC Metals

Y. Kogure and T. Kosugi*

Teikyo University of Science & Technology, Uenohara, Yamanashi 409-01, Japan

**Hiroshima University, Higashi Hiroshima, Hiroshima 739, Japan*

Abstract. Motion of dislocations was studied by means of molecular dynamics simulation. The embedded atom method (EAM) potential is used to express the non-central nature of atomic interaction in metals. A new EAM potential expressed by simple functions has been developed and used in the simulation. The equilibrium configuration of atoms and the motion of dislocations in Cu and Ag crystals were carefully investigated. From the change of the kinetic energy and the position of the dislocation, the Peierls potential was estimated.

1. INTRODUCTION

In the molecular dynamics study of dislocations a choice of interatomic potential is very important because it affects the structure and the motion of dislocations. In metals and alloys the importance of the many body interaction due to the conduction electrons are recognized, and the embedded atom method (EAM) potential has been developed [1-3]. We have been developed a new EAM potential, which is expressed by simple functions and can be applied efficiently to the molecular dynamics simulation. The potential is used in the present study.

The Peierls potential in fcc metals is considered to be very small, but the magnitude is not well understood. The computer simulation may be a useful method to clarify the Peierls potential and the motion of dislocations.

2. EMBEDDED ATOM METHOD POTENTIAL

Many types of the embedded atom method potential functions have been proposed [1-3] to express the atomic interactions in metals. A new potential function developed by the present authors has been used in the simulation.

$$E_i = F(\rho) + \frac{1}{2} \sum_{j \neq i} \phi(r_{ij}), \quad (1)$$

where the electron density function is expressed as

$$F(\rho_i) = D \rho_i \ln \rho_i, \quad \rho_i = \sum_{j \neq i} f(r_{ij}). \quad (2)$$

Functions $\phi(r)$ and $f(r)$ are

$$\phi(r) = A(r_c - r)^2 \exp(-c_1 r), \quad (3)$$

$$f(r) = B(r_c - r)^2 \exp(-c_2 r). \quad (4)$$

Where r_{ij} is the distance between atom i and j . r_c is a cut off distance of the potential. r_{ij} and r_c are normalized by the nearest neighbour distance. It is noted that the first derivatives of $\phi(r)$ and $f(r)$ are 0 at $r = r_c$. Namely, the potential is smoothly truncated. These functions contain

Table I. EAM potential paremeters.

	A [eV]	B	C_1	C_2	D [eV]	r_c
Cu	6200.7	0.019609	11.128	0.42223	13.389	1.955
Ag	935.96	0.11751	8.6974	2.4203	14.231	1.970

Table II. Calculated physical values.

	a [Å]	c_{11}	c_{12}	c_{44}	E_c [eV]	E_v [eV]	E_s [erg/cm ²]
Cu	3.61496	1.803	1.206	0.714	3.54	1.32	71.1
		(1.684)	(1.214)	(0.754)	(3.54)	(1.30)	(74)
Ag	4.0862	1.254	0.929	0.459	2.85	1.10	6.7
		(1.240)	(0.934)	(0.461)	(2.85)	(1.10)	(17)

(Values in parentheses are experimental values, and the values of ealstic constants are in units of 10^{12} dynes/cm²)

Figure 1: Configuration of atoms after initial relaxation. Split dislocation is seen.

five parameters, A , B , C_1 , C_2 , and D . The parameters are determined by fitting the functions to the experimental values of the cohesive energy E_c , the lattice constant a , the elastic constants (c_{11} , c_{12} , c_{44}) and the formation energy of the vacancy E_v . The determined values of the parameters are summarized in Table I. The elastic constants and other energies calculated from these parameters are compared with the experimental values in Table II. The potential function has been used in the simulation of the melting and the glass transition.

3. METHOD OF SIMULATION

The motion of a straight screw dislocation in copper and silver crystals is considered. The slip plane is $\{111\}$, the slip direction is $\langle 110 \rangle$, and the dislocation line is directed along $\langle 110 \rangle$. Two sizes of model crystals with 1392 or 3666 atoms rows are used for the simulation. As an initial condition, atoms in the model crystal are displaced following to the strain field given by the elasticity theory of the dislocation. Then the crystals are relaxed through the molecular dynamics. To obtain an equilibrium configuration, the crystal is quenched by setting the velocities of all atoms to zero. The quenching is made when the total kinetic energy of the atomic system attain a maximum. An example of the equilibrium configuration after the initial relaxation is shown in Figure 1, where the two atomic plane adjacent to the dislocation line are separately shown by solid and open circles in Fig. a). The Burgers vector density shown below is the finite derivative of the relative displacement

Figure 2: Change of Burgers vector density in Cu and Ag under a stress $\tau = 4 \times 10^{-4} \mu$.

at the slip plane, by which the position of the dislocation can be seen clearly. It is seen that the dislocation is split to partials and a stacking fault between the partial dislocations is shown by a dashed line in b).

After the initial relaxation the shear stresses were applied and the motion of the dislocation was monitored through the Burgers vector density. The time interval for the molecular dynamics was chosen as 5×10^{-15} sec, and the equilibrium configuration was obtained after 3000 time steps.

4. RESULTS AND DISCUSSION

The motion of split dislocations in Cu and Ag under an external stress $\tau = 4 \times 10^{-4} \mu$ is shown in Figure 2, where μ is the shear modulus. A value S denotes the number of molecular dynamics time steps. At $S = 0$ dislocations are in equilibrium. It is seen that the width of a split dislocation is larger in Ag than in Cu. This may be due to the difference of stacking fault energy (E_s in Table II). According to the elasticity theory, the repulsive force F between two partials separated by a distance r is given by $F = a^2 \mu / 24 \pi r$. Here, a is the lattice constant. The force balances the stacking fault energy γ in equilibrium state. Then the distance is

$$r = a^2 \mu / 24 \pi \gamma. \quad (5)$$

The stacking fault energy of Cu calculated from the present potential is 73 erg/cm² and the distance r is estimated to be 17 - 26 Å, which is consistent with the result of simulation, 18 Å. In the case of Ag, the distance calculated by eq. (5) is about three times larger than the observed one. This may be due to the back force from the crystal surfaces, because the simulation is done under the fixed boundary condition.

As the time steps S increases the dislocations start to move. It is seen that the split partials moves together in Cu, and that the partials moves one by one in Ag. The partials in Ag are widely spread and they may be able to move more freely than in Cu.

Figure 3: Change of total kinetic energy.

The total kinetic energy of atoms involved in the simulation E_{KE} is calculated at every time step. A result under the stress $\tau = 4 \times 10^{-4} \mu$ is shown in Figure 3. The energy increases with the number of time steps and a small dip is seen at $S = 300 - 400$ in the case of Cu. As the total energy is conserved during the molecular dynamics, the decrease of the kinetic energy corresponds to the increase of the potential energy. By comparing this with the change of the Burgers vector density the increase of the potential energy is considered to be due to the Peierls potential energy, and the Peierls stress for the dislocation in Cu is estimated to be $2 - 3 \times 10^{-5} \mu$. There are no such dips in the result of Ag, and the Peierls stress of a dislocation in Ag is anticipated to be small. A more detailed investigation in a larger model crystal is in progress.

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