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Molecular dynamics study of self-diffusion in the core of a screw dislocation in face centered cubic crystals

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ABSTRACT

Self-diffusion along the screw dislocation core in aluminum, nickel, copper and silver in the absence of any pre-existing point defects in the structure is studied using molecular dynamics. Simulation results show that the effect of screw dislocation on enhancing self-diffusion is more remarkable in Al and Ni than in Cu, and no significant enhancement of self-diffusion has been observed in the core regions of Ag. This behavior has been related to higher stacking fault energies and resultant smaller dissociation distance of partial dislocations in Al and Ni, compared to Cu and Ag.

Enhanced diffusivity in the core region of lattice dislocations have been reported for a number of crystalline materials including Al, Cu, Ag, Ni [1,2]. Fast diffusion along dislocation core, also known as pipe-diffusion, has been shown to have a significant role in controlling the kinetics of many processes such as creep [3], precipitate coarsening in precipitation-strengthened alloys [4,5], solute segregation to surfaces [6,7] and sintering [8]. Despite the importance of pipe diffusion, there is a lack of understanding about the underlying mechanisms of this phenomenon. Experimental studies on pipe diffusion are mainly based on tracer diffusion along low angle tilt boundaries [1,9,10], and only a few studies are available on isolated dislocations [11]. On the other hand, simulation studies are mainly focused on diffusion along edge dislocations by introducing a point defect (vacancy or interstitial) in the core and following the migration path and based on the assumption that diffusion is only mediated by atomic exchanges with the point defect [12,13]. Three mechanisms have been proposed that can contribute to diffusion in the core regions in FCC metals: vacancy [11], interstitial [14] and intrinsic mechanism [15]. Vacancy and interstitial mechanisms have been associated with lower formation or migration energies of these point defects in the core with respect to the bulk [1,12,16], indicating that diffusivity along dissociated dislocations decreases as the degree of dissociation into partial dislocations increases. For intrinsic diffusion (diffusion without any pre-existing point defects), no comprehensive mechanism has been suggested. Pun and Mishin [15] have confirmed the existence of intrinsic diffusion in core regions of aluminum, an FCC metal with high stacking fault energy (i.e. small dissociation distance of partials). However, the existence of intrinsic diffusivity, especially in FCC metals with low stacking fault energy and resultant high dissociation distance of partials, remains unclear.

The purpose of the present study is to investigate the existence of self-intrinsic-diffusion along screw dislocation core in FCC metals, and analyze the relation between stacking fault energy and diffusivity along the dislocation core. Identifying the effect of stacking fault energy and corresponding dissociation distance of partials on the extent of pipe-diffusion is of particular interest, due to the importance of this phenomenon on dictating kinetics of various processes in materials. To achieve the above objective, diffusion behavior in dislocation containing single crystals with different level of stacking fault energies is studied through Molecular Dynamics (MD) simulations.

MD simulation is performed using LAMMPS package [17] and embedded atom method (EAM) potentials. Simulation studies have been conducted on four FCC metals: aluminum, nickel, copper and silver. These metals are selected because of their high (i.e. Al and Ni), medium (i.e. Cu) and low (i.e. Ag) stacking fault energies. The EAM potentials used for these elements are described in [18–21] and accurately predict the values of stacking fault energies and activation energies of bulk diffusion for the chosen metals, as reported in Table 1. Melting temperatures predicted using these potentials are 1042 K for Al, 1715 for Ni, 1327 K for Cu and 1267 K for Ag.

In order to study self-diffusion along a screw dislocation core in each of these elements, a cylindrical model with periodic boundary

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Table 1
Calculated separation distance of dislocations (d), pipe-diffusion activation energy (E_d), integrated diffusion flux (P_d^0) and pre-exponential factor of pipe-diffusion (D_d^0). Stacking fault energies (E_{stk_flt}) and bulk diffusion activation energies (E_b) are obtained from EAM potentials [18–21].

Element	$E_{stk_{flt}}$ (mJ m^{-2})	d (Å)	E_b (eV)	E_d (eV)	P_d^0 (cm^{4}s^{-1})	D_d^0 (cm^{2}s^{-1})	E_d/E_b
Al	146 [18]	7	1.2 [18]	0.57	2.3×10^{-18}	2.1×10^{-4}	0.48
Ni	134 [21]	9	2.76 [21]	1.58	5.9×10^{-17}	5.3×10^{-3}	0.57
Cu	45 [19]	13	1.96 [19]	1.61	4.6×10^{-16}	4.1×10^{-2}	0.82
Ag	17 [20]	25	1.76 [20]	–	–	–	–

conditions along the z axis is created. Axes x, y and z are parallel to $[\bar{1}\ 1\ \bar{2}]$, $[\bar{1}\ 1\ 1]$, and [110] crystallographic directions, respectively. The cylinder has the length of about 50 Å and diameter of about 150 Å. The approach described in [22] is used to create a dislocation along the z direction. All atoms are displaced from their initially perfect lattice positions according to the isotropic linear elasticity solution for a straight screw dislocation [23] with the Burgers vector ½ [110]. According to this theory, for a straight screw dislocation, the only non-zero component of the displacement vector $u = (u_x, u_y, u_z)$ is u_z and it depends only on the x and y coordinates of the field point $X = (x,y,z)$ [22]:

$$u_z\,(x,y) = b\,\frac{\theta}{2\pi} \tag{1}$$

where b is the Burgers vector and $\theta \in (-\pi, \pi]$ is the angle between the vector connecting the origin to $(x,y,0)$ and the x axis. A smaller cylinder is cut out from this cylinder, with the same length and a smaller diameter of about 80 Å. Atoms within a 10 Å thick outer layer of this cylinder are fixed and all other atoms are relaxed at 0 K using the conjugate gradient method implemented in LAMMPS. In all four cases of Al, Ni, Cu and Ag, the dislocation dissociates into Shockley partials on a {111} plane. However in Al, the dissociation width is very narrow and the distance between partial dislocations is only about 7 Å (about 2.5b), whereas the dissociation widths for Ni, Cu and Ag are about 9 Å (about 3.5b), 13 Å (about 5b) and 25 Å (about 8.5b), respectively. These values follow the general fact that the degree of dissociation increases with decreasing stacking fault energy and are in agreement with earlier experimental and simulation results [24,25]. In order to efficiently perform MD runs with a small number of atoms, more atoms on the outer layer of the cylinder are fixed. Free atoms are located in a cylinder with a diameter of about 30 Å to 50 Å, depending on the element under study. Diffusion has been studied at constant temperatures between 800 K to 1000 K for Al, 1500 K to 1600 K for Ni and 1250 K to 1325 K for Cu. A series of MD runs close to melting point, 1267 K, are also performed for Ag. With respect to the chosen temperature, the simulation box is expanded uniformly before MD runs in order to minimize the thermal stresses at high temperatures. Using the NVT (constant number of particles, volume and temperature) ensemble and a time step of 2 femtoseconds, the temperature is increased to the chosen value during the first 1 ns followed by an isothermal annealing for 30 ns to 60 ns, depending on the temperature and the element understudy. It should be emphasized that no vacancy (or interstitial) is introduced into the system; therefore any diffusion at high temperatures is related to the intrinsic diffusion.

In order to describe diffusion along the dislocation core, the dislocations are often represented as high diffusivity pipes embedded in a lower diffusivity matrix. The diffusivity is related to the structure of the dislocation core, which in turn is dictated by the magnitude of Burgers vector, the direction of the dislocation line and the stacking fault energy [1]. It is only possible to obtain values of the combined parameter [1]

$$P_d = D_d A_d \tag{2}$$

where P_d is the integrated diffusion flux, D_d is the diffusivity along dislocation core and A_d is the effective cross-sectional area of dislocation core. By analogy to bulk diffusion, the following equation has been used for pipe-diffusion [1]

$$D_d = D_d^0\ exp\left(-\frac{E_d}{kT}\right) \tag{3}$$

where E_d is the activation energy for diffusion along dislocation core and D_d^0 is the temperature independent pre-exponential factor. The value of E_d is typically 0.6–0.7 of the activation energy of bulk diffusion, whereas D_d^0 is close to typical values for bulk diffusion [2]. In experimental measurements, it is usually assumed that fast diffusion occurs only in the inelastic region of the dislocation core, often a cylindrical pipe of radius $r_d = 5$ Å [1].

The results of MD simulations are analyzed following the method proposed in [15] to find D_d^0 and E_d in Eq. (3). Isothermal annealing time is divided into 10 shorter time intervals. For each interval, imaginary cylinders with radii R, ranging from 5 Å to 13 Å centered at midpoint between partials are chosen. To find the diffusion coefficient in each cylinder, Mean-Squared Displacements (MSD) along the

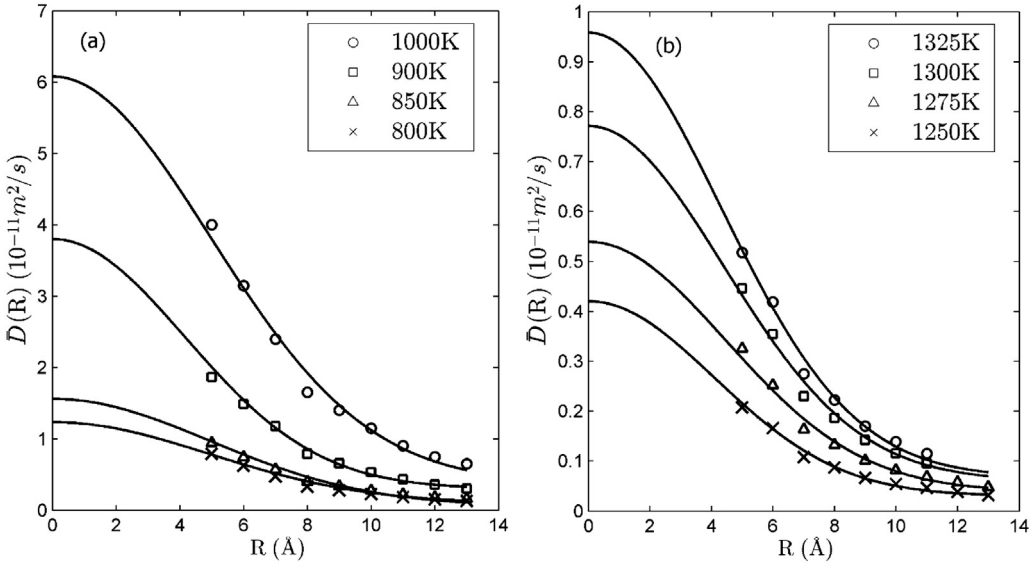

Fig. 1. Average dislocation diffusivity vs. radius R for (a) Al and (b) Cu. Each data point is calculated using Eq. (4) and curves are fitted to Eq. (5).