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Mechanism of intrinsic diffusion in the core of screw dislocations in FCC metals – A molecular dynamics study

Siavash Soltani [a], Niaz Abdolrahim [b], Panthea Sepehrband [a,*]

[a] *Department of Mechanical Engineering, Santa Clara University, Santa Clara, CA 95053, United States*
[b] *Department of Mechanical Engineering, University of Rochester, Rochester, NY 14604, United States*

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ABSTRACT

The mechanism of self-diffusion in the absence of any pre-existing point defects (intrinsic diffusion) along an a/2 ⟨1 1 0⟩ screw dislocation in FCC metals is studied using molecular dynamics simulations. High diffusivity along the dislocation core at elevated temperatures is found to be due to the constriction of partial dislocations, where a vacancy-interstitial pair forms. The two point defects separate and start to migrate along the core, giving rise to diffusion. Formation energy for both vacancy and self-interstitial are found to be much lower on the constricted node of partial dislocations compared to other atomic sites, indicating the important role of the constriction in enhancing the diffusion.

1. Introduction

It has been established that diffusivity of atoms in the core regions of dislocations is much higher than in surrounding lattice regions [1]. Although the effect of high diffusivity paths provided by dislocation cores on enhancing the kinetics of many diffusion-controlled processes in FCC metals has been extensively reported [2–4], the diffusion mechanisms acting in core regions and their extent of contribution to diffusivity remains debated. Since the vacancy mechanism is the most energetically favorable diffusion mechanism in bulk, it has been suggested as the main mechanism of fast diffusivity along the dislocation core [1]. Interstitials have also been proposed to considerably contribute to fast diffusivity along the core [5]. Huang et al. [6] found the activation energy of self-diffusion along the dissociated edge dislocations in Cu to be about 1.82 eV through interstitial mechanism and about 1.72 eV through vacancy mechanism (the activation energy of self-diffusion in bulk Cu is about 2.72 eV and 2.24 eV through interstitial and vacancy mechanisms, respectively [6]). Using an MD approach Von Boehm and Nieminen [7] showed when both vacancies and self-interstitial exist, the interstitial mechanism would be the dominant mechanism of self-diffusion along dissociated edge dislocations in Au. More recently, Pun and Mishin [8] revealed the existence of another mechanism for diffusion along the dislocation core in Al: “the intrinsic mechanism.” Intrinsic diffusivity corresponds to enhanced diffusion along the core in the absence of any pre-existing point defects. It is revealed that when an equilibrium number of vacancies and self-interstitials are introduced into the core regions, their contributions to diffusion will be negligible compared to the intrinsic diffusion [8].

In our recent work [9], we investigated the existence of intrinsic self-diffusion along a full a/2 ⟨1 1 0⟩ screw dislocation in four FCC metals (Al, Ni, Cu and Ag) with various level of stacking fault energies. No point defects were introduced into the system; therefore, any diffusion was due to intrinsic diffusion. At high temperatures, enhanced diffusion was observed along the dislocation core in all materials, except in Ag. Enhanced self-diffusion was found to be more remarkable in Al and Ni compared to Cu, and occurrence of diffusion through the intrinsic mechanism was suggested to be related to the dissociation distance between partials, which is affected by the stacking fault energy of the crystal. Al and Ni have high stacking fault energies and a low dissociation width of partial dislocations, while Cu has a medium level of stacking fault energy and a medium dissociation width. By quantifying the activation energy of diffusion, it was found that the diffusivity weakens as the distance between the two partials increases. Since it was observed that the two Shockley partials are able to frequently reverse (constrict) at high temperatures in Al, Ni and Cu, it was suggested that high diffusivity along the core might be due to the constriction of partials. Even at high temperatures, no diffusion was observed in the core regions of Ag that has low stacking fault

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* Corresponding author.
E-mail address: psepehrband@scu.edu (P. Sepehrband).

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energy. This has been related to the very high dissociation width of partial dislocations in Ag, making the interaction and constriction of partial dislocations an unlikely event. Although the recent studies [8,9] show the existence of intrinsic diffusion, the mechanism remains unknown.

The purpose of the present work is to define the mechanism of intrinsic self-diffusion along a screw dislocation in FCC single crystals. For this purpose, i) generation of point defects and their migration paths in core regions are analyzed, ii) the role of constricted partial dislocations on enhanced diffusivity is identified through computing the vacancy formation energy on different atomic sites (i.e. on partial dislocations, in stacking fault ribbon, and on the constricted node of partial dislocations) and the results are compared with the values of vacancy formation energy in bulk.

2. Point defect generation in the dislocation core

To investigate the intrinsic diffusion and its mechanism, a single full $a/2[1\,1\,0]$ screw dislocation, is created in FCC crystals of Al, Ni, Cu and Ag, using molecular dynamics and LAMMPS package [10]. A cylindrical model is defined for each of the materials, based on the approach implemented in [9]. Axis x is along $[\bar{1}\,1\,\bar{2}]$, y and z axes are along $[\bar{1}\,1\,1]$ and $[1\,1\,0]$ crystallographic directions, respectively. The diameter and length of the cylinder are about 60 Å and 50 Å respectively. Periodic boundary conditions are implemented along z axis. EAM potentials used in this study for Al, Ni, Cu and Ag are described in [11–14]. Linear elasticity solution [9,15] for a straight screw dislocation is used to create a full dislocation with $\mathbf{b} = 1/2[1\,1\,0]$ at the center of the cylinder and along z axis. Atoms within 10 Å thick outer layer of the cylinder are fixed to restrict the dislocation escape from the system. Upon relaxations, the full $a/2\,\langle 1\,1\,0\rangle$ dislocation dissociates into two Shockley $a/6\,\langle 1\,1\,2\rangle$ partial dislocations in all four elements. The distance between the partials is about 7 Å (about 2.5**b**) in Al, about 9 Å (3.5**b**) in Ni, about 13 Å (5**b**) in Cu, and about 25 Å (8.5**b**) in Ag. As expected, the dissociation width is larger in Cu and Ag, which is due to their lower stacking fault energies compared to Al and Ni. As an example, the relaxed structure of Al, at 0 K, is shown in Fig. 1(a). The temperature is then increased to a target value (below the melting point) and is kept constant using NVT (constant number of atoms, volume and temperature) ensemble and a time step of 2 fss for several nanoseconds. It should be emphasized that no point defects is introduced in the structures.

At high temperatures (in all elements, except in Ag), two important phenomena are detected in the dislocation core regions: (i) constriction of partial dislocations, as shown in Fig. 1(b) and (ii) formation and migration of vacancy-interstitial pairs, Fig. 2. The point defects are identified using Wigner-Seitz defect analysis tool implemented in Ovito [16]. In this method, each atom in the reference configuration defines the center of a Wigner-Seitz cell, which is the spatial region belonging to that site. Any atom from the displaced configuration (which is any snapshot of the structure during the annealing) that is located within the Wigner-Seitz cell of a reference site is said to occupy that site. The modifier then outputs the number of atoms occupying a site.

As shown in Fig. 2, most of the sites are identified to be occupied by one atom (color coded with white). However, it is observed that at some snapshots, there are sites occupied by zero atoms (e.g. vacancy formation, color coded with blue) and some sites are also occupied by two atoms (e.g. self-interstitial formation, color coded with red). Since no point defect has been introduced in the initial structure, this observation suggests that at high temperatures, the dislocation core becomes an effective source for point defect generation. Pairs of vacancy and self-interstitial that form in the core regions of Al at 1000 K are shown in Fig. 2(a). The two point defects either recombine immediately, or separate and migrate along the core and give rise to diffusion, as shown in Fig. 2(b). After migration along the core, the vacancy and self-interstitial come into vicinity of each other again (Fig. 2(c)) and recombine to restore the defect-free structure. The formation, migration and recombination of pairs take a fraction of picoseconds. Fig. 2(d) shows formation of several vacancy-interstitial pairs in core regions. Formation and migration of vacancy-interstitial pairs have been observed only for the materials in which constriction of the two partial dislocations occurs (i.e. Al, Ni, and Cu). These observations imply that the formation and migration of point defects in core regions is related to the constriction of partial dislocations. Generation of vacancy-interstitial pairs in core regions in Al has been also reported by Pun and Mishin [8].

3. Point defect formation energy

Since the state of minimum energy for a set of atoms is normally obtained by their perfect crystal structure, it is possible to estimate the location of the crystal defects using the potential energy per atom [17]. Since the cohesive energy of Al using this potential is −3.36 eV, any atom in the perfect FCC positions in Al should have a potential energy of −3.36 eV. Using this quantity,

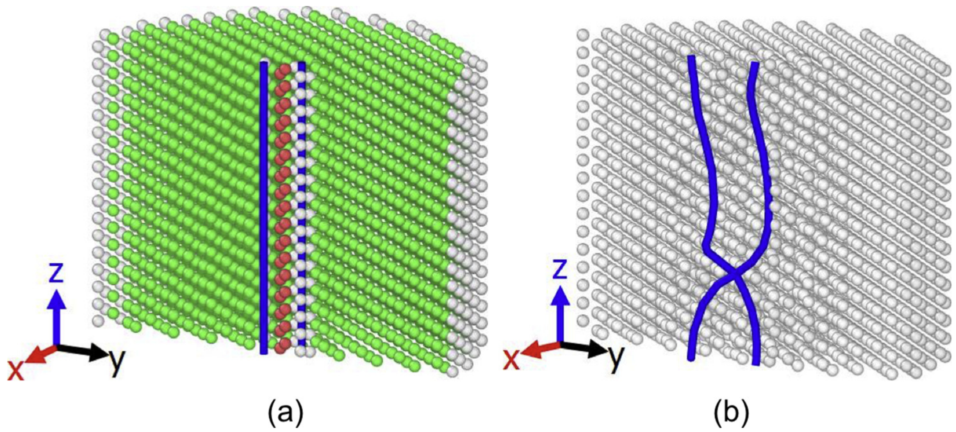

Fig. 1. A slice of the cylinder. (a) Relaxed structure of Al at 0 K, color coded using common neighbor analysis. Green and red color represent FCC and HCP structures, respectively. Blue segments show partial dislocations. Atoms in the vicinity of partial dislocations have neither FCC nor HCP structure. (b) Reversion and constriction of partial dislocation in Al at a random snapshot at 900 K. Dislocations are extracted using DXA method implemented in OVITO [16]. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)