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A molecular dynamics study of self-diffusion in the cores of screw and edge dislocations in aluminum

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Abstract

Self-diffusion along screw and edge dislocations in Al is studied by molecular dynamics simulations. Three types of simulations are performed: with pre-existing vacancies in the dislocation core, with pre-existing interstitials, and without any pre-existing defects (intrinsic diffusion). We find that diffusion along the screw dislocation is dominated by the intrinsic mechanism, whereas diffusion along the edge dislocation is dominated by the vacancy mechanism. Diffusion along the screw dislocation is found to be significantly faster than diffusion along the edge dislocation, and both diffusivities are in reasonable agreement with experimental data. The intrinsic diffusion mechanism can be associated with the formation of dynamic Frenkel pairs, possibly activated by thermal jogs and/or kinks. The simulations show that at high temperatures the dislocation core becomes an effective source/sink of point defects and the effect of pre-existing defects on the core diffusivity diminishes.

Keywords: Dislocation; Diffusion; Vacancy; Interstitial; Computer simulation

1. Introduction

The mobility of atoms in core regions of lattice dislocations can be orders of magnitude higher than in surrounding lattice regions. For historic reasons, this phenomenon is often referred to as “pipe diffusion”, although it should properly be called “dislocation diffusion” for consistency with the well-established terms of grain boundary diffusion and surface diffusion [1–3].

The fast atomic transport along dislocations can play a significant role in the kinetics of many processes in materials [4]. Dislocation diffusion can contribute to creep mechanisms, including dislocation climb and Orowan loop bowing [5]. Deviations from the power law of creep can be attributed to dislocation diffusion [6,7]. Diffusion of solute atoms along arrested dislocations is one of the proposed mechanisms of dynamics strain aging in alloys exhibiting flow instabilities [8–10]. The kinetics of solute segregation to surfaces and grain boundaries can be enhanced by diffusion along dislocations terminating at the interfaces [11–13]. Coarsening kinetics in precipitation-strengthened alloys are often influenced or even controlled by dislocation diffusion, especially in nanometer-scale structures in which dislocation lines can directly connect the growing particles. Diffusion along misfit dislocations at γ/γ' interfaces can contribute to the γ'-phase coarsening and rafting kinetics, affecting the creep resistance of superalloys [14]. Dislocation diffusion can influence sintering processes [15–17], oxidation, corrosion, recovery of radiation damage, and electromigration damage in microelectronic devices [18].

Despite its importance, the phenomenon of dislocation diffusion is not well understood on the fundamental level. The amount of reliable experimental information is rather limited [1–3]. According to experimental data available, the coefficient D_d of dislocation diffusion approximately follows the Arrhenius law

$$D_d = D_d^0 \exp\left(-\frac{E_d}{k_B T}\right), \qquad (1)$$

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k_B being the Boltzmann constant and T temperature. The activation energy of dislocation diffusion, E_d, is approximately 0.6–0.7 of the activation energy of lattice diffusion E, whereas the pre-exponential factor D_d^0 is close to typical values for lattice diffusion [1]. Dislocation diffusion coefficients tend to increase with the magnitude of the Burgers vector and decrease with the dissociation width into Shockley partials in face-centered cubic metals. It is assumed that dislocation diffusion is mediated by atomic exchanges with single vacancies, although there is no convincing experimental evidence for this mechanism. In fact, except for the analogy with lattice diffusion, there is no fundamental reason why vacancy diffusion must necessarily dominate over interstitial diffusion or other possible diffusion mechanisms.

Experimental measurements of dislocation diffusion are difficult and can be divided in two categories. In *direct* measurements, the diffusion coefficient is extracted from the penetration profile (concentration vs. depth) of radioactive tracer or impurity atoms diffused into a deformed single crystal or a polycrystal containing low-angle grain boundaries. The penetration profile is analyzed in terms of continuum models, in which the dislocations are represented by high-diffusivity "pipes" of some radius r_d whose diffusion coefficient D_d is much larger than the lattice diffusivity D. Several mathematical solutions of this diffusion problem have been developed [3], all assuming that the dislocations are normal to the surface and arranged in a wall or another (e.g., hexagonal) periodic array. By fitting a model solution to the experimental profile, the so-called integrated diffusion flux $P_d = D_d A_d$ is extracted, where $A_d = \pi r_d^2$ is the cross-sectional area of the dislocation "pipe". To estimate D_d separately, an assumption about r_d must be made, which is usually $r_d = 0.5$ nm. This uncertainty of r_d does not affect applications since it is only the quantity P_d that appears in all models of diffusion-controlled processes in materials, not D_d separately. Most of the dislocation diffusion coefficients available today were measured in the 1960–1970s. Very few direct measurements are made these days, see [19] (radiotracer self-diffusion in Fe) and [20,21] (secondary-ion mass spectrometry for oxides) as some recent examples.

In *indirect* methods, P_d is back-calculated from the rate of a particular diffusion-controlled process, such as internal friction, dislocation climb, dislocation loop shrinkage, phase growth kinetics [22,18], or annihilation of dislocation dipoles [1,23,21]. Essentially, it can be any process whose rate is assumed to be controlled by dislocation diffusion and for which a model containing P_d is available. Unfortunately, such models often rely on crude approximations and contain other unknown parameters. Indirect measurements are only accurate up to an order of magnitude at best and have a poor reproducibility.

As one example relevant to this work, Table 1 summarizes experimental data for Al self-diffusion. For dislocation diffusion, only indirect measurements from void-shrinkage kinetics are available [24]. For dislocation diffusion in Al alloys, only crude estimates of the activation energy from internal friction experiments [25] exist in the literature.

The enhanced atomic mobility along dislocations and the correlation $E_d \approx 0.6 - 0.7E$ were confirmed by early atomistic simulations with pair potentials [26–28]. Contrary to the common assumption, Huang et al. [27,28] found that vacancies and interstitials could make comparable contributions to dislocation diffusion. More accurate simulations employing embedded-atom method (EAM) potentials have recently been performed for dislocations in Au [29], Al [30–33,4] and Cu [27–29], as well as Al–Mg [33] and Al–Cu [34] alloys. The rates of vacancy jumps along the core were found to depend on the dislocation character (edge, screw or mixed). However, except for [4,29], only diffusion by the vacancy mechanism was analyzed. Furthermore, while the diffusion coefficient of vacancies, D_v, was calculated in several studies [28–31], the atomic diffusion coefficient D_d was only estimated in Refs.

Table 1
Summary of experimental data for the pre-exponential factor D_0 and activation energy E of lattice diffusion, grain-boundary diffusion, and dislocation diffusion in Al. δ is the grain boundary width and A_d is the cross-sectional area of the dislocation core. The dash indicates that data is unavailable.

	Lattice diffusion		Boundary diffusion		Dislocation diffusion	
	D_0 (m^2/s)	E (eV)	δD_{0b}(m^3/s)	E_b (eV)	$A_d D_{0d}$ (m^4/s)	E_d (eV)
Lundy and Murdock [51]	1.71×10^{-4}	1.47	–	–	–	–
Volin et al. [24]	–	–	–	–	7.0×10^{-25}	0.85
Engardt and Barnes [52]	–	1.3	–	–	–	–
Spokas and Slichter [53]	–	1.40	–	–	–	–
DeSorbo and Turnbull [54]	–	1.44	–	–	–	–
Fradin and Rowland [55]	3.5×10^{-6}	1.25	–	–	–	–
Stoebe and Dawson [56]	0.02×10^{-4}	1.22	–	–	–	–
Stoebe and Dawson [56]	1.7×10^{-4}	1.48	–	–	–	–
Häßner [57]	–	–	1.9×10^{-14}[a]	0.62	–	–
Gangulee and d́Heurle [58]	–	–	2.3×10^{-22}	–	–	–
Levenson [59]	–	–	–	0.55	–	–
Haruyama et al. [60]	–	–	–	–	–	0.90
Federighi [61]	–	1.33	–	–	–	–
Volin and Balluffi [62]	1.76×10^{-5}	1.31	–	–	–	–

[a] 1.9×10^{-5} m^2/s multiplied by $\delta = 1.0$ nm.