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Effect of saddle point anisotropy of point defects on their absorption by dislocations and cavities

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ABSTRACT

Developing predictive models for the microstructure evolution of materials requires an accurate description of the point defects fluxes to the different sinks, such as dislocations, grain boundaries and cavities. This work aims at improving the evaluation of sink strengths of dislocations and cavities using object kinetic Monte-Carlo simulations parametrized with density functional theory calculations. The present accurate description of point defects migration enables quantitative assessment of the influence of the point defects anisotropy at saddle point. The results in aluminum show that the anisotropy at saddle point has a large influence on sink strengths. In particular, this anisotropy leads to the cavity being a biased sink. These results are explained by the analysis of the point defect trajectories to the sinks, which are shown to be strongly affected by the saddle point anisotropy.

1. Introduction

Supersaturation of point defects in metals occurs, for example, after plastic deformation [1], hydrogen charging [2,3], solid or liquid state quenching [4–6] and irradiation [7]. This supersaturation leads to the formation of vacancy clusters such as voids, stacking fault tetrahedra and dislocation loops and, in the case of irradiation, self-interstitial clusters. These clusters are sinks for point defects and grow, thereby affecting the macroscopic properties of materials.

Fluxes of point defects to the sinks of the microstructure strongly depend on the elastic field created by the sinks, which modify the energy landscape. Striking examples of the role of elastic interactions between sinks and point defects on the final microstructure come from materials under irradiation. Swelling [7] and irradiation creep [8,9] are due to a slight imbalance of absorption of point defects (self-interstitial atoms (SIAs) and vacancies) by the different sinks of the microstructure. In the so-called “dislocation bias model”, swelling is due to the preferential absorption of interstitials by dislocations, which is responsible for a net flux of vacancies to cavities [10]. In this model, cavities are assumed to be neutral sinks, which means that they have no absorption bias for interstitials. Some models for irradiation creep, such as SIPA (Stress Induced Preferred Absorption), rely on the difference in climb velocity of different dislocation populations, depending on their orientation with respect to the applied stress. In such models, the climb velocity depends not only on the applied stress, but also on the stress field created by the dislocations [8]. In order to simulate irradiation induced phenomena such as swelling and creep, a proper description of the effect of the elastic field created by sinks on point defect migration is therefore crucial.

The simulation of long term microstructures under irradiation is conveniently performed by rate equation cluster dynamics [11–14]. In this kind of mean-field model, the variation of the migration energy along the point defect trajectory cannot be taken into account explicitly. The effect of elastic interactions on point defect diffusion is found in the sink strengths for SIAs (k_i^2) and vacancies (k_v^2). The bias, which is defined as the relative difference between the sink strengths k_i^2 and k_v^2, quantifies to what extent a sink preferentially absorbs SIAs or vacancies, depending on its sign.

A large amount of data exists about sink strengths and bias values, but the scattering is rather high. Assuming that dislocations are the only biased sinks, the dislocation bias can be inferred from experimental swelling data, using standard rate theory models [15–19]. However, swelling is a combination of the bias and the fraction of freely migrating defects, which is not precisely known for ion and neutron irradiations. Therefore, there is some

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uncertainty about the bias values obtained by such methods. Depending on the experimental data and the assumptions of the rate theory model, the dislocation bias values typically range between 0.01 and 0.35. Sink strengths and biases can also be computed. A common way is to solve the drift-diffusion equation for the concentration of point defects around a sink. This method was used for the first calculations, mostly for simple geometries and simple description of the sink–point defect interaction [20–23]. For more complex cases, phase field [24] and object kinetic Monte-Carlo (OKMC) simulations have been used [25–27]. OKMC methods are particularly handy to take into account the effect of elastic interactions at stable and saddle points [28,29].

The influence of elastic interactions at saddle position on the value of sink strength was emphasized by Dederichs and Schroeder [30]. Although this effect had been discussed previously [31–33], these authors also suggested that the *anisotropy* of point defects at saddle position could have an effect on the sink strength. Such an effect was later confirmed for straight dislocations [34–37], infinitesimal dislocation loops [38] and voids [39]. However, all these works contain approximations to make calculations tractable, so the values of sink strengths significantly vary from one study to the other [37]. In addition, the elastic dipoles of point defects are based on empirical potential calculations, which are not always in agreement with first-principles calculations. Only recently, the effect of saddle point anisotropy has been shown for the sink strength of semi-coherent interfaces, using OKMC simulations parameterized with density functional theory (DFT) calculations [29].

In the present work, we perform OKMC simulations to study the sink strengths of straight dislocations and spherical cavities in pure aluminum, in order to assess the role of saddle point anisotropy. To that purpose, the elastic interactions between sinks and point defects are modeled explicitly in the OKMC code. Point defects are represented by their elastic dipole tensors computed by DFT calculations.

This paper is structured as follows. Section 2 describes the method used to calculate sink strengths. Section 3 presents the study of the straight dislocation. The case of a spherical cavity is treated in section 4.

2. Methods

2.1. OKMC simulations and sink strength calculation

Sink strengths are calculated with an OKMC code [29], allowing the simulation of many point defect trajectories in an efficient way, and making it possible to account for the point defects properties and elastic interactions between point defects and sinks [28,29,40]. A single type of sink is introduced in the simulation box. It can be a dislocation or a spherical cavity. The sinks are considered as immobile and remain unchanged after absorption of defects. The temperature is set to 300 K. At this temperature, thermal equilibrium concentration of point defects is far smaller than the concentration imposed by irradiation. Therefore, thermal generation of point defects by the sinks is neglected.

SIAs and vacancies are considered separately, in dedicated simulations, thus no recombination is possible. They are generated uniformly at a constant creation rate G_0 (in s^{-1}), and migrate inside the box by performing atomic jumps until they are absorbed by the sink. The migrating point defects do not react with each other to form clusters and no long-range interactions between point defects are considered. Periodic boundary conditions are used in all 3 dimensions. Point defects are considered as absorbed by the sink when the distance d between the sink center and the point defect verifies $d \leq d_{\text{reac}}$ where d_{reac} is the reaction distance depending on the nature of the sink.

To increment the simulation time, a residence time algorithm is used [41,42]. At a given time t, the time step is given by $\Delta t = -\ln(r_1)/\Gamma_{\text{tot}}$ where r_1 is a random number chosen in $]0,1]$ and Γ_{tot} is the sum of the frequencies of all N_e possible events, *i. e.* $\Gamma_{\text{tot}} = \sum_{i=0}^{N_e-1}\Gamma_i$. The possible events are the creation of a point defect due to irradiation (frequency $\Gamma_0 = G_0$) or an atomic jump from a stable position to a neighboring one (frequency Γ_i, $i = 1, \ldots, N_e - 1$). The chosen event j is such that $\sum_{i=0}^{j-1}\Gamma_i < r_2\Gamma_{\text{tot}} \leq \sum_{i=0}^{j}\Gamma_i$, with r_2 a random number chosen in $]0,1]$. Frequencies of atomic jumps are given by $\Gamma_i = \nu_0 \exp(-\Delta E_i/(k_B T))$, with ν_0 the attempt frequency assumed to be the same for all jumps, k_B is the Boltzmann constant, T the temperature and $\Delta E_i = E_i^{\text{sad}} - E_i^{\text{sta}}$ the difference of energy between the saddle point of the jump and the initial stable position.

The energy of point defects at stable point E_i^{sta} and at saddle point E_i^{sad} are given by

$$E_i^{\text{sta}} = -\sum_{j,k} P_{i,jk}^{\text{sta}} \varepsilon_{jk}(\boldsymbol{r}_i^{\text{sta}}) \tag{1}$$

$$E_i^{\text{sad}} = E^{\text{m}} - \sum_{j,k} P_{i,jk}^{\text{sad}} \varepsilon_{jk}\left(\boldsymbol{r}_i^{\text{sad}}\right), \tag{2}$$

where E^{m} is the migration energy without elastic interactions and $\boldsymbol{P}^{\text{sta}}$ and $\boldsymbol{P}^{\text{sad}}$ are elastic dipole tensors (**P**-tensors) describing the point defects at stable and saddle positions, respectively [43,44]. The saddle position $\boldsymbol{r}^{\text{sad}}$ is simply considered as the midpoint along the reaction coordinate between the two stable positions involved in the jump. The strain, written $\boldsymbol{\varepsilon}$, is generated by the sink. Since we focus on the effect of saddle point anisotropy, we consider that **P**-tensors do not depend on the local strain, *i. e.* we neglect polarisability effects [43]. Other energy terms, such that higher order terms in the multipole expansion [44] and image interactions for voids [45,46], are also neglected.

In our simulations, unless otherwise specified, the calculations are performed in isotropic elasticity, using available analytical expressions of the strain produced by the sink. This assumption is expected to be reasonable in the case of face centered cubic (FCC) aluminum, studied here, because the elastic moduli tensor of this material is only weakly anisotropic (see Table 1). This makes it possible to focus on the effect of point defects anisotropy only. However, to check the influence of the anisotropy of the elastic moduli tensor on the sink strength, simulations are also performed in anisotropic elasticity, using the values of elastic constants given in Ref. [47]. In that case, a Fast Fourier Transform (FFT)-based method is used to compute the strain field at mechanical equilibrium [48–50].

In the mean field rate theory, the sink strength k^2 defines the ability of a sink to absorb point defects. In this formalism, the evolution equation of the average number of defects $\overline{N}$ is given by

Table 1
Elastic constants of aluminum at 300 K. The isotropic elastic constants are calculated from the tensor terms by the Voigt average [51].

Elastic moduli tensor terms and Zener anisotropy ratio [47]			
C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	$A = 2C_{44}/(C_{11} - C_{12})$
106.51	60.38	27.8	1.21
Constants for isotropic elasticity			
Poisson's ratio ν			Shear modulus μ (GPa)
0.35			25.91