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Multiscale calculations of dislocation bias in fcc Ni and bcc Fe model lattices

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ABSTRACT

In order to gain more insights on void swelling, dislocation bias is studied in this work. Molecular static simulations with empirical potentials are applied to map the dislocation–point defects interaction energies in both fcc Ni and bcc Fe model lattices. The interaction energies are then used to numerically solve the diffusion equation and obtain the dislocation bias. The importance of the dislocation core region is studied under a the temperature range 573–1173 K and the dislocation densities 10^{12} – 10^{15} m^{−2}. The results show that larger dislocation bias is found in the fcc Ni than in the bcc Fe under different temperatures and dislocation densities. The anisotropic interaction energy model is used to obtain the dislocation bias and the result is compared to that obtained using the atomistic interaction model, the contribution from the core structure is then shown in both the Ni lattice and the Fe lattice.

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1. Introduction

Radiation induced swelling is one of the primary issues in development of new types of nuclear power plants. This issue severely restricts the lifetime of structural materials in nuclear reactors. The micro-structure evolution of the material under irradiation is the key for understanding the phenomenon of radiation induced swelling [1]. It is well known that a biased absorption of self interstitial atoms (SIA) by dislocations is crucial for void swelling under high temperature and high radiation dose. This biased absorption is described by the dislocation bias factor (B_d). The parameter quantifies the preferential absorption of SIAs, compared to absorption of vacancies, by dislocations. It is regarded as the intrinsic driving force for void swelling in the standard rate theory model [2,3]. In this model, only Frenkel pairs (FPs) are considered and therefore excess vacancies are absorbed by voids. In the more sophisticated production bias model [4], however, production and annihilation of the primary clusters and their functions as sinks and sources of point defects are properly taken into account. Dislocation bias is still an integral part even of this complex model. In spite of its importance, dislocation bias has not yet been fully understood mainly because no direct

experimental measurement is available. Instead, the bias factor could be derived from other experimental values, given a certain swelling model. Meanwhile, theoretical studies derived from elasticity theory have been used to obtain the bias factor [5]. The theoretical predictions, however, do not give any quantitative agreement with the experimental derived values [6]. One of the insufficiencies regarding the theoretical approach is the simplified interaction energy models of dislocation and point defects (PDs). Due to the complicated mathematical characterization of a defect migrating in the strain field of a dislocation, it is difficult to find an analytical solution to the diffusion equation with a drift term. However, a few important solutions were obtained. The fundamental one is Ham's solution. In that model, only the first order size interaction was considered in an isotropic material [5]. Improvements have been made by including also the effects of modulus interactions [7]. However, the fundamental characterization, such as the anisotropy and SIA dumbbell orientations, are not complete. In this work, atomistic simulations made in a comparably large model crystal lattice have been used to obtain the interaction energy of dislocation and PDs for both fcc (Ni) and bcc (Fe) lattices. With the information from atomistic calculation, a numerical method has been applied to obtain the dislocation bias. The contribution from the dislocation core structure on dislocation bias has been discussed and the influences of temperature and dislocation densities have been reported.

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2. Theory

2.1. Isotropic interaction

The interaction energy is an important input parameter to obtain the dislocation bias. With a infinite, straight edge dislocation, the interactions between dislocation and point defects could be described by a continuum model. In this model, the interaction arises from the coupling between the long-range stress field of a dislocation and the atomic displacements around the point defect. The crystal is treated as an isotropic elastic medium, and point defects are modeled as elastic inclusions. Assuming that the point defects are perfectly spherical, the interaction energy between dislocation and point defects described by the isotropic elasticity theory can be written as [8]

$$E = -A \frac{\sin \theta}{r} \quad (1)$$

where

$$A = \frac{\mu b}{3\pi} \frac{1+\nu}{1-\nu} |\Delta| \quad (2)$$

in polar coordinates (r, θ) . μ is the shear modulus, ν is Poisson's ratio, b is the Burgers vector, and, Δ is the relaxation volume of the PD.

This isotropic elastic expression originates from the interaction between the strain fields of dislocation and PDs, in which the distortion produced by the edge dislocation is regarded as an elastic distortion of a cylindrical ring. Although this approach is often used for the analytical calculation of the bias factor, the intrinsic isotropic assumption is a limit for its application.

2.2. Anisotropic interaction

In this model we consider the case where the xy -plane is a plane of symmetry. Then the problem is considerably simplified. The anisotropic stress field of the edge dislocation in a cubic crystal is obtained from [9]:

$$\sigma_{11} = \frac{-b}{2\pi} I \frac{y[(3+H)x^2 + y^2]}{(x^2 + y^2)^2 + Hx^2y^2} \quad (3)$$

$$\sigma_{22} = \frac{b}{2\pi} I \frac{y(x^2 - y^2)}{(x^2 + y^2)^2 + Hx^2y^2} \quad (4)$$

$$\sigma_{12} = \frac{b}{2\pi} I \frac{x(x^2 - y^2)}{(x^2 + y^2)^2 + Hx^2y^2} \quad (5)$$

$$I = (c_{11} + c_{12}) \left[\frac{c_{44}(c_{11} - c_{12})}{c_{11}(2c_{44} + c_{11} + c_{12})} \right]^{1/2} \quad (6)$$

and

$$H = \frac{(c_{11} + c_{12})(c_{11} - c_{12} - 2c_{44})}{c_{11}c_{44}}. \quad (7)$$

where c_{ij} are elastic constants. For a cubic crystal, only three of these coefficients remain independent, eg: c_{11} , c_{12} and c_{44} .

The effective pressure acting on a volume element is [10]:

$$p = -\frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33}) \quad (8)$$

where $\sigma_{33} = \nu(\sigma_{11} + \sigma_{22})$ is the same as it is in the isotropic case. Therefore the interaction energy $E = p|\Delta|$ is written as:

$$E = \frac{b(1+\nu)I}{6\pi} |\Delta| \frac{(2x^2y + Hx^2y + 2y^3)}{(x^2 + y^2)^2 + Hx^2y^2}. \quad (9)$$

This expression converges to the isotropic case Eq. (1) when $c_{44} = \frac{c_{11}-c_{12}}{2}$ is applied.

3. Method

3.1. Computational method

In order to calculate the interaction between a dislocation and a PD, large model lattices are constructed by using semi-empirical embedded atom method (EAM) potentials for Ni [11] and Fe [12]. In fcc Ni, a $\langle 110 \rangle \{111\}$ edge dislocation is generated while in bcc Fe, a $\langle 111 \rangle \{110\}$ is constructed. The simulation box of Ni is $70a_0 \times 7a_0 \times 76a_0$ in the $[110]$, $[-11-2]$ and $[-111]$ directions, respectively. The simulation box of Fe is $100a_0 \times 3a_0 \times 67a_0$ in the $[111]$, $[11-2]$ and $[-110]$ directions, respectively. Both simulation boxes are large enough to exclude the image interaction from the periodic boundary conditions.

The dislocations are introduced in the center of the model lattices in the same way as Osetsky et al. [13]. Two orientations of $\langle 100 \rangle$ dumbbells and six orientations of $\langle 110 \rangle$ dumbbells are inserted as different configurations to fully describe the interaction of the dislocation with the SIAs in Ni and in Fe lattices, respectively. Calculations are made for cases of PDs in different lattice sites on the plane that includes the Burgers vector and cutting perpendicular to the dislocation line. Full relaxation of the model lattices are performed by a static method using the DYMOKA code [14]. During the relaxation of the dislocation line, fixed boundary conditions are applied on the $[-111]$ and $[-110]$ directions for Ni and Fe respectively, while periodic boundary conditions are used on the Burgers vector directions and the dislocation line directions. The total energies of the whole lattice are then calculated as a function of lattice site coordinates between a PD and a dislocation.

3.2. Bias calculation method

The diffusion of a PD in a stress field can be described by Fick's law with a drift term:

$$J = -\nabla(DC) - \beta DC \nabla E \quad (10)$$

with J the flux of point defects, D the diffusion coefficient, C the concentration of the point defects, $\beta = 1/k_B T$ with k_B the Boltzmann constant and T the temperature, and E the interaction energy of the dislocation with the point defects. The concentration of defects $C(r)$ satisfies the steady-state diffusion equation around the sink:

$$\nabla \cdot J = 0 \quad (11)$$

By rewriting it into a diffusion potential form:

$$\nabla^2 \Psi = \beta \nabla E \cdot \nabla \Psi \quad (12)$$

where $\Psi = DCe^{\beta E(r,\theta)}$ is referred to as the diffusion potential function, this partial differential equation is solvable with certain boundary conditions.

In our case, it is assumed that all point defects are absorbed at the dislocation core region. Hence the boundary condition at the dislocation core $r = r_0$, is $\Psi_{r_0} = 0$. At the external boundary, i.e. the dislocation radius of influence, $r = R$, the defect concentration $C(r, \theta)$ is a constant and the interactions vanish. Hence, $\Psi_R = C^{\text{eq}}$ where C^{eq} is the concentration of point defects in the steady state.

Assuming a straight dislocation with a core of cylinder shape, the flux of PDs reaching unit length of a dislocation is evaluated as [15]:

$$J_{\text{tot}} = r_0 \int_0^{2\pi} J_r(r_0, \theta) d\theta \quad (13)$$

where r_0 is the dislocation core radius, $J_r(r_0, \theta)$ is the current to the core.

The dislocation capture efficiency Z in this case is defined as the ratio of point defects fluxes with and without the interaction term E , i.e. $Z = \frac{J}{J_0}$, where J_0 is the flux excluding the interaction contribution. Furthermore, the dislocation bias is defined as

$$B_d = \frac{Z_{\text{SIA}}}{Z_{\text{vac}}} - 1. \quad (14)$$

The numerical solution of Eq. (12) is based on a finite element method (FEM), which has been implemented in the MATLAB PDE-toolbox. Finite elements are used to discretize the partial differential equation, resulting in a group of linear functions. Those linear functions are then solved by an iterative approach on a pre-defined geometry area. The area has been meshed by numerous nodes, the solution on each node gives the diffusion potential of PDs on that point, from which the flux can be calculated. The total flux J_{tot} is then integrated on the dislocation inner radius.

4. Results and discussion

4.1. Method analysis

In order to assess the precision of the numerical method, dislocation capture efficiencies are calculated from both continuum-mechanical model and the numerical method. The former is an explicit solution of Eq. (12) using Eq. (1) [15]:

$$Z = \frac{2\pi I_0(L/2r_0)}{K_0(L/2R) \cdot I_0(L/2r_0) - K_0(L/2r_0) \cdot I_0(L/2R)} \quad (15)$$

where r_0 is the dislocation core radius and R is the external boundary where $E(R) = 0$. L is well known as the interaction range:

$$L = \frac{\mu b}{3\pi k_b T} \frac{1+v}{1-v} |\Delta| \quad (16)$$

Note that Eq. (16) and Eq. (2) differ only by a factor of $\frac{1}{k_b T}$.

The results are shown in Table 1. All calculations are performed with $r_0 = 5 \text{ \AA}$ and $T = 873 \text{ K}$. The numerical results overestimate the capture efficiencies to some extent. The overestimation is probably due to the sample meshes that is used in the numerical method. In our previous study [16], it has been shown that the more sample meshes we use, the more precisely the partial differential equation is solved. However, the more sample meshes we use, the more expensive in terms of computational time it is. We here take a balance between the precision and the computational time by using 128 points on the dislocation inner radius. A maximal deviation of about 4% between the numerical results and the continuum-mechanical model occurs on Z_{SIA} when $R = 100 \text{ \AA}$. This R is comparable to a dislocation density of 10^{16} m^{-2} . As the external boundary R increases, that is, the dislocation density decreases, the error decreases. On the other hand, Z_{SIA} retains a larger discrepancy than Z_{vac} under all listed dislocation densities. Thus, it is reasonable to conclude that a higher interaction energy or a higher dislocation density results in a higher over estimation. For the calculations

in this paper, the dislocation core radius is selected so that the average interaction energy on the core is 0.113 eV, which corresponds to the thermal fluctuation threshold at the temperature of 873 K. Therefore, r_0 in Ni is 22 Å while r_0 in Fe is 15 Å. Moreover, all comparisons are performed under the same dislocation density.

4.2. Interaction energies

In fcc Ni lattice two partial dislocations are observed after full relaxation. The distance between the partial dislocations is about 22 Å, which is reasonable judging from the stacking fault energy of 113 mJ/m². Two SIA dumbbells, namely [100] and [001], are introduced. The average of the two dumbbells interaction energy is used in the dislocation bias calculations. On the other hand, there are 6 different orientations of $\langle 110 \rangle$ dumbbells in bcc Fe. The same average procedure is used as well. The average SIA–dislocation interaction energy along the z-direction, which is perpendicular to the plane formed by the Burgers vector and the dislocation line, through the center point is shown in Fig. 1. The elastic model refers to the anisotropic elastic model. It retains a symmetric interaction energy in compressive field and the tensile field, while in the atomistic model, there is a higher interaction energy in the compressive field side. This is reasonable because the formation energy of an SIA is higher in the compressive side of the dislocation than in the tensile side. By comparing the dislocation–SIA interaction in bcc and fcc lattices, a more localized interaction in bcc Fe is noticed, see Fig. 1. This could be explained by the relative small and non-split dislocation core in bcc lattices.

4.3. Bias factor calculation

The dislocation bias factors have been calculated under different temperatures and different dislocation densities in both Ni and Fe. Figs. 2 and 3 shows the influence of temperature on the dislocation bias factors. Dislocation bias decreases as the temperature increases in both cases. This is in line with our previous work [17]. The diffusion of PDs is more active at higher temperatures, hence the drift term is less effective in the high temperature range. This is the reason for the smaller difference between B_d calculated from the atomistic model and from the elastic models at higher temperature where diffusion is dominant. Since the diffusion model does not take into account any point defect clusters, no peak swelling

Fig. 1. Interaction energy along the direction that is perpendicular to the plane formed by the Burgers vector and the dislocation line. The 0.113 eV is $3k_b T/2$ at the temperature $T = 873 \text{ K}$.

Table 1

Calculations of capture efficiencies from the isotropic continuum-mechanical model (CMM) and the numerical solution.

R (Å)	Z_{vac}		Z_{SIA}	
	CMM	Numerical	CMM	Numerical
100	1.0291	1.0335	1.1646	1.2011
200	1.0237	1.0248	1.1309	1.1428
300	1.0213	1.0271	1.1167	1.1172
400	1.0199	1.0239	1.1083	1.1159
500	1.0184	1.0194	1.1025	1.1097

Fig. 2. Dislocation bias as a function of temperature in bcc Fe.

Fig. 3. Dislocation bias as a function of temperature in fcc Ni.

profile is observed as temperature varies. Given the fact that the Zener's elastic anisotropy factor $A = \frac{2C_{44}}{C_{11} - C_{12}}$ is 2.5 in Ni and 2.3 in Fe, both are highly anisotropic. The isotropic model is not appropriate in describing the dislocation–PD interaction in these model lattices. Therefore the anisotropic interaction energies are used to calculate the dislocation bias using the same numerical method. The difference between the bias calculated from anisotropy interaction model and atomistic interactions are due to the exact dislocation core structure. It is shown from the two figures that the relative difference between the atomistic calculation and the numerically solved elastic models are larger in the bcc Fe comparing to it in the fcc Ni. This might due to the partial dislocation separation in the fcc Ni. Further more, the dislocation bias in Ni is higher than in Fe in all cases demonstrated in Figs. 2 and 3. This is in line with Kuramoto et al. [18]. Considering the computational cost, that is, about 1500 core hours for each interaction map which contains $1.5 \cdot 10^5$ atoms, it is, therefore, much lighter to obtain the bias from the elastic interaction energies. Thus, at relatively high temperature and low dislocation density, the elastic interaction energies might be sufficient to obtain an approximate dislocation bias in the Fe, Ni and Cu [17] cases. However, one should be careful

Fig. 4. Dislocation bias as a function of dislocation density in fcc Ni and bcc Fe.

when using the elastic interaction model to estimate the dislocation bias on other metals, because the different elastic constants and stacking fault energies could play important roles in the interaction energy and dislocation bias calculations.

The influence of dislocation densities are also studied. As shown in Fig. 4, B_d increases as the dislocation density increases. The rate of increase depends on the dislocation density. In general, a higher density refers to a higher B_d rate.

5. Summary and conclusions

Atomistic calculated interaction energies are used here to numerically solve the diffusion equations that describes a point defect migrating in a dislocation strain field in bcc Fe and fcc Ni. Dislocation bias factors are thus obtained. A general conclusion is that larger dislocation bias is found in fcc Ni than in bcc Fe, which is in qualitative agreement with experiment. The possible reason is that the dislocation core range in bcc is much smaller than in fcc. Various temperature and dislocation density conditions are used to analyze the influences on dislocation bias in different model lattices. A simple positive correlation has been found for B_d and the dislocation density while a negative correlation has been found with respect to temperature. The anisotropic elastic interaction energy model is compared to the atomistic model, demonstrating that the effect of the dislocation core structure is non-negligible.

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