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

Z. Chang [a,*], P. Olsson [a], D. Terentyev [b], N. Sandberg [c]

[a] Reactor Physics: Royal Institute of Technology KTH, Stockholm, Sweden
[b] SCK-CEN, Nuclear Materials Science Institute, Mol, Belgium
[c] Swedish Radiation Safety Authority, SSM, Solna, Sweden

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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.

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 insufficies 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.

* Corresponding author.
E-mail address: zhongwen@kth.se (Z. Chang).

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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]

$$E = -A\frac{\sin\theta}{r} \tag{1}$$

where

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

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]:

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

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

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

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

and

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

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]:

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

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:

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

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 $70a_0 * 7a_0 * 76a_0$ in the [1 1 0], [−1 1 −2] and [−1 1 1] directions, respectively. The simulation box of Fe is $100a_0 * 3a_0 * 67a_0$ in the [1 1 1], [1 1 −2] and [−1 1 0] 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 [−1 1 1] and [−1 1 0] 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:

$$J = -\nabla(DC) - \beta DC\nabla E \tag{10}$$

with J the flux of point defects, D the diffusion coefficient, C the concentration of the point defects, $\beta = 1/k_BT$ 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:

$$\nabla\cdot J = 0 \tag{11}$$

By rewriting it into a diffusion potential form:

$$\nabla^2\Psi = \beta\nabla E\cdot\nabla\Psi \tag{12}$$

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, $\Psi_R = C^{eq}$ 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]:

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