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3D phase-field modelling of dislocation loop sink strengths

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ABSTRACT

This work presents a 3D phase-field model to correctly evaluate dislocation loop sink strength. This method is applied to a wide range of microstructures (dislocation loops of various types with isotropic or anisotropic elasticity, like in Zr, cohabitation of different types of loop in the same calculation domain), which allows to exhibit several original results. Among them, in the case of isotropic elasticity, our model shows that the sink strength of vacancy loops is higher than that of interstitial ones for low loop radii. In the case of Zr, the effect on sink biases of the shape anisotropy of self-interstitial atoms, already exhibited in the case of straight dislocations, is enhanced for loops and stabilizes basal vacancy and prism-plane interstitial ones. Moreover, isotropic elastic interactions promote the coexistence of parallel vacancy and interstitial loops. This result is still valid in the case of prism-plane loops in Zr, which could provide explanations to several experimental facts.

1. Introduction

The standard rate theory (SRT) [1–3] was devised to describe microstructure evolution under irradiation. It is a mean field theory, which in spite of its rather simple assumptions, is able to explain a large variety of observed phenomena under irradiation. SRT assumes for instance that interstitial atoms (SIAs) and vacancies are produced at the same amount (Frenkel pairs). Such assumption is reasonable for electron irradiation for instance, but it is known to be simplistic in the case of damage production by cascades at the end of which interstitials have tendency to cluster instead of remaining isolated. This effect was taken into account by the production biased model which in its most recent versions assumes that interstitial clusters are mobile [4,5].

Whatever the nature of the produced interstitials (isolated or clusters), the capacity of a given element of the microstructure to absorb them preferentially rather than vacancies, the so-called sink bias, remains a crucial parameter which must be accurately determined to predict microstructure evolution under irradiation. Regarding the nature of the sinks, it is known that the bias associated to voids B_c, which have rather smooth elastic interactions with point defects (PDs), is small and is often neglected [6]. On the other hand, the bias associated to dislocations B_d is known to be of prime importance for instance to describe swelling: according to the SRT, the steady-state swelling rate is determined by the void distribution and is proportional to B_d if B_c is neglected (see Ref. [7] for instance).

In between voids and straight dislocations, dislocation loops do have a strong elastic interaction with PDs that may lead to a significant bias B_{dl}. The contribution of B_{dl} can be significant since many metallic alloys under irradiation develop a high density of prismatic dislocation loops. The theoretical determination of B_d and B_{dl} is generally made assuming that close to the line cores, the PD concentration is fixed at its thermal equilibrium value (perfect sink assumption). The dislocation lines and PDs interact through long-range elastic interactions and the boundary conditions adopted most of the time are of the Dirichlet type (imposing a fixed concentration far from the lines without considering a bulk PD creation rate) for sake of analytical resolution. However, in real situations, the boundary conditions are close to zero PD fluxes between the attraction basins of neighboring sinks. The Dirichlet condition has recently been shown to significantly underestimate B_d [8]. In addition, analytical solutions are often limited to isotropic cases (defects are considered as dilatation centres moving in an isotropic elastic medium). The case of B_{dl} is still more complicated due the higher topological intricacy and therefore less literature is available concerning it. In most analytical works, a solution to this problem is proposed under the assumption that the loop is elastically equivalent to a spherical sink [9,10].

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The true toroidal geometry of the loop has been numerically considered in the work of Dubinko et al. [11] in the case of isotropic elastic and diffusional properties. They showed in particular that the choice of the sink-free volume shape can strongly affect the calculated sink strengths. This illustrates the interest of considering numerical methods with no topological constraints, like the Object Kinetic Monte Carlo method (OKMC) described in Ref. [12]. In this framework, Jansson et al. [13] computed sink strength of dislocation loops in order to specifically investigate the effect of diffusion anisotropy, but without considering elastic interactions that are known to be important especially for SIAs.

Recent calculations of B_d based on atomic-scale modeling [14,15] have shown the necessity to take into account the atomic-scale interactions between PDs and dislocation cores to correctly evaluate B_d. The core effect seems to be stronger for bcc rather than for fcc metals and concerning the sink strength, the core effect is more pronounced for interstitials than for vacancies. Pointing out the importance of this core interactions, the atomistic calculations have nevertheless intrinsic limitations and the methodology used make also cumbersome the study of sinks with complicated topologies. These works also pointed out the necessity to correctly describe elastic interactions which introduce first-order corrections to the bias calculations, like in Refs. [16,17].

In previous works [8], a phase-field approach was proposed to perform B_d calculations. The employed methodology was lately used to determine B_d for anisotropic materials like hcp Zr [18]. It allowed to emphasize the effect of the shape anisotropy of SIAs (SAS) to correctly evaluate the biases associated to the various types of dislocations observed in Zr. It was also shown that this effect was consistent with the coexistence of basal vacancy loops and interstitial prism-plane loops. The application domain of the method has then been extended to determine B_{dl} [19], which allowed to assess the validity of the analytical solutions for loops proposed so far. The purpose of this paper is to extend this previous work and to determine the loop sink strength in presence of elastic interactions, including specific cases for which (i) anisotropic elastic interactions between PDs and loops and (ii) multiple sink effects are expected. This is the case for Zr alloys which develop vacancy and interstitial loops in prismatic planes and vacancy loops in basal planes under irradiation.

The article is divided as follows: we start by a description of the phase-field model and we then calibrate it using 3D sinks for which strength values are known. The model is then applied to study the sink strength of dislocation loops in elastically isotropic materials. Since an exhaustive study of anisotropic elasticity is not possible, hcp Zr has been chosen as an application example for which the different types of loops observed experimentally under irradiation are treated. The case of elastically interacting interstitial and vacancy loops is specifically studied and discussed, and allows to exhibit original and unexpected results concerning their mutual stabilization.

2. Methodology

2.1. Phase-field model

The generalization of the PF model presented in Ref. [8] to several types of loop is straightforward. 3 types of order parameter are required:

- The PD site fraction field $X(\mathrm{r})$ interacting with dislocations. PDs are created by irradiation at a uniform and constant generation rate K_0, and absorbed locally by the dislocation cores. Only Frenkel pairs are considered ($X(\mathrm{r})$ refers either to vacancies or SIAs).
- The shape function $\eta_{dl}(\mathrm{r})$ of the dislocation loop of type dl, equal to 1 for any point located inside the loop and 0 outside. This non-conserved order parameter allows to define the local eigenstrain associated to the loop. In our case, a disk-shaped platelet of centre c_{dl} and radius $r_{L,dl}$ is considered, hence, the dislocation is a circular loop the border of which overlaps with the core of the dislocation line (Fig. 1 a)). In the basis (x,y,z), the habit plane of the loop is always chosen parallel to (xy), hence η_{dl} is defined as follows:

$$\eta_{dl}(\mathrm{r}) = \delta(z - z_{c,dl})\frac{1}{2}\left[1 - \tan h\left(\frac{\sqrt{(x-x_{c,dl})^2 + (y-y_{c,dl})^2} - r_{L,dl}}{\sqrt{2}\,W}\right)\right] \quad (1)$$

where (x,y,z) and $(x_{c,dl},y_{c,dl},z_{c,dl})$ are respectively the coordinates of r and centre c_{dl}, $W = 2a_0$, a_0 being the size of the PF cell, $\delta(0) = 1$ and $\delta(x \neq 0) = 0$. According to Eq. (1), the value of η_{dl} changes sharply from 0 to 1 in the direction normal to the habit plane, while in any direction in the habit plane, η_{dl} increases smoothly from its minimal to maximal value.

- The order parameter $\lambda_{dl}(\mathrm{r})$ reproduces the sink behaviour of the dislocation. It is equal to 0 in the matrix and 1 in the capture zone of the sink, defined as a torus of centre c_{dl}, major radius $r_{L,dl}$ and minor radius $r_{0,dl}$ (Fig. 1 b)). The (x,y,z) coordinates of any point located inside the torus verify:

$$\left[r_{L,dl} - \sqrt{(x-x_{c,dl})^2 + (y-y_{c,dl})^2}\right]^2 + (z-z_{c,dl})^2 < {r\prime}_{0,dl}{}^2 \quad (2)$$

It must be emphasized that $\eta_{dl}(\mathrm{r})$ and $\lambda_{dl}(\mathrm{r})$ are defined consistently, i.e. the dislocation core (border of the platelet η_{dl}) is fully embedded inside the sink toroidal region λ_{dl} (Fig. 1 c)).

In the following, two types of calculation domains are considered. Due to periodic boundary conditions, the first one, represented in Fig. 1 c), depicts a periodic lattice constituted of one type of loop (dl=1) of centre ($N/2\,a_0$, $N/2\,a_0$, $N/2\,a_0$), N being the number of cells in each direction. In Fig. 1 d), the size of the domain is doubled in the direction perpendicular to the habit plane of the loop in order to contain two different types of loop (dl=1 or 2) centered on c_1 ($N/2\,a_0$, $N/2\,a_0$, $N/2\,a_0$) and c_2 ($N/2\,a_0$, $N/2\,a_0$, $3N/2\,a_0$): this type of simulation is a first step towards a real investigation of interacting microstructural defects, which can allow to reveal unknown multi-sink effects on sink strength calculations.

The free energy functional F is expressed as:

$$F = F^{chem}(X) + E^{el}(X,\eta_{dl}) + E^{core}(\eta_{dl}) \quad (3)$$

F^{chem} is the chemical free energy of the system, E^{el} is the elastic energy and E^{core} is the core energy of the dislocation lines. If we consider the defect-free crystal as the reference, then the excess chemical free energy of the system of volume V due to the point defect fraction $X(\mathrm{r})$ is given by Ref. [20]:

$$F^{chem} = \frac{1}{V_{at}}\int_V E_f X(\mathrm{r}) + k_B T[X(\mathrm{r})\ln(X(\mathrm{r})) + (1 - X(\mathrm{r}))\ln(1 - X(\mathrm{r}))]\cdot dV \quad (4)$$

V_{at} is the atomic volume, E_f is the PD formation energy, k_B is the Boltzmann constant and T is the temperature of the system. This expression can be obtained assuming either a constant number of