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Quantitative phase field model for dislocation sink strength calculations

H. Rouchette [a], L. Thuinet [a,*], A. Legris [a], A. Ambard [b], C. Domain [b]

[a] Unité Matériaux Et Transformations (UMET), UMR CNRS 8207, Université Lille 1, 59655 Villeneuve D'Ascq, France
[b] EDF R&D MMC, Électricité de France, 77810 Moret-sur-Loing, France

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ABSTRACT

An original phase-field model dedicated to the calculation of dislocation sink strength is presented. Through a three-step validation procedure, it is shown to predict with an excellent accuracy the value of the sink strength with or without elasticity in numerous test cases for which an analytical solution is known. Further analysis shows that existing analytical values of dislocation sink strength are significantly underestimated, an effect that results from simplifying assumptions made to take into account irradiation in the diffusion equation.

1. Introduction

Materials submitted to continuous radiation are maintained in nonequilibrium conditions that may accelerate their microstructure evolution and/or and induce unexpected structural bifurcations [1]. In the case of metallic alloys at relatively low temperature, radiation produces points defects (PDs) in quantities overwhelmingly larger than those expected at thermal equilibrium. PDs annihilate and/or are absorbed by microstructural defects called sinks (dislocation lines, dislocation loops, voids, grain boundaries, heterophase interfaces, etc.). The ability of sinks to absorb PDs is of primary importance to determine microstructure evolution, since sinks may grow during irradiation and induce structural changes like swelling, shrinkage, radiation growth or radiation induced creep. In a metallic material containing an average atomic fraction $\bar{X}_i^{RT}$ of point defect i at steady state, the rate of absorption J_i^s by a sink of type s and density ρ_s is assumed to follow a second order reaction law [2–4]:

$$J_i^s = Z_i^s \rho_s D_i (\bar{X}_i^{RT} - X_i^s), \tag{1}$$

with D_i the diffusion coefficient of species i, X_i^s the concentration of i at the surface of the sink (supposed in general to be equal to its thermal equilibrium value X_i^{th}) and Z_i^s the sink efficiency. The sink strength corresponds to $Z_i^s \rho_s$. Eq. (1) is used in rate theory (RT) simulations to predict the evolution of $\bar{X}_i^{RT}$ on long time scale.

Analytical expressions have been proposed for sink efficiency obtained after resolution of the diffusion equation of PDs around the considered sink using different boundary conditions [2]. To this end, it is necessary to define a reservoir, i.e. a representative average volume around the sink and free of any other microstructural defect. The main parameters influencing the capture efficiency are then: (i) the geometry and volume of the sink, (ii) the geometry and volume of the reservoir, (iii) the properties of the diffusion tensor (isotropic/anisotropic) of the species and (iv) the existence or not of a diffusion drift generated for instance by an elastic stress gradient. In general, two spatial parameters are introduced, namely the sink radius or width r_0 and the radius or width of the reservoir R (typically the mean distance between sinks) that is related to the sink density ρ_s. Assuming simple situations (isotropic diffusion and no elasticity), a compilation of Z_i^s expressions can be found in [2].

At this stage, it is important to emphasise that for a given sink, the choice of the boundary conditions can lead to different expressions of Z_i^s. In principle, J_i^s should be established assuming the PD production rate as a source term in the diffusion equation (model of Poisson) and imposing a constant PD fraction $X_i^s = X_i^{th}$ at r_0. If instead the solution of the diffusion equation is obtained without a production term (Laplace equation) by choosing correctly the boundary values $X_i(R)$ and X_i^s, the values of Z_i^s are different from those obtained from the Poisson equation, this difference being more pronounced for a 1D (dislocation line) than for a 3D (voids) microstructural defects. The latter approach is more employed since it is easier to solve analytically [2] (see Table 1 for Poisson's and Laplace's expressions).

The previous results were extended to the case of diffusion anisotropy [5]. In this case, it is possible to obtain an analytical

* Corresponding author. Tel.: +33 (0) 320 33 62 25; fax: +33 (0) 320 43 65 91.
E-mail addresses: Hadrien.Rouchette@ed.univ-lille1.fr (H. Rouchette), Ludovic.Thuinet@univ-lille1.fr (L. Thuinet).

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Table 1
Description of the different analytical models with their boundary conditions (BC), sink efficiency Z and flux expression J^s.

	Laplace	Poisson	Wiedersich
Equation	$D\nabla^2 X = 0$	$D\nabla^2 X + K_0 = 0$	$D\nabla^2 X + K_0 = 0$
BC	$X(r_0) = X^{th}$	$X(r_0) = X^{th}$	$X(r_0) = X^{th}$
	$X(R) = X^{th} + \frac{K_0 R^2 \ln(R/r_0)}{2D}$	$\frac{\partial X}{\partial r}(R) = 0$	$\frac{\partial X}{\partial r}(R) = 0$
Z	$\frac{2\pi}{\ln(f_d^{-1/2})}$	$\frac{2\pi}{\ln(f_d^{-1/2}) + \frac{1}{2}f_d - 1)}$	$\frac{2\pi(1-f_d)}{\ln(f_d^{-1/2}) - \frac{3}{4} + \frac{1}{4}f_d(4-f_d)}$
J^s	$Z^{Lap} D\rho_d (X(R) - X^{th})$	$Z^{Pois} D\rho_d (X(R) - X^{th})$	$Z^{W} D\rho_d (\bar{X} - X^{th})$

expression of Z_i^s by solving the Laplace equation. As an application, it was shown that a difference in diffusion anisotropy (DAD) between vacancies and self-interstitial atoms (SIAs) can induce a sink absorption bias that could explain the radiation growth of non-cubic irradiated materials. None of the approaches previously mentioned takes into consideration elastic effects, an approximation which is not accurate when dealing with sinks generating significant stress fields, such as dislocations. However, getting an analytical expression for the sink strength that properly takes into account the diffusion drift generated by elastic fields is very challenging, and so far, most of the works dedicated to such calculations assumed elastically isotropic systems. Under this assumption, Ham [6] derived an exact solution of the sink strength for edge dislocations. Wolfer and Ashkin [7,8] developed a perturbation method to handle point defects as elastic inhomogeneities, i.e. with different elastic constants from the matrix but still isotropic, which allows them to study the effect of an applied stress on the sink strength. Their work showed a stress-induced preferred absorption of defects (SIPA) and provides a physical basis to explain irradiation creep. Dubinko et al. [9] calculated numerically the sink strength of a dislocation loop by solving the diffusion equation with elasticity in a toroidal reservoir. This work emphasises the importance of the reservoir topology (toroidal vs spherical) on the resulting sink strength. It is important to note that all these developments were made using the same boundary conditions than those used to solve the Laplace equation mentioned previously.

To take into account sink morphologies that deviate from simple reference cases but also interactions between adjacent sinks, numerical methods have been developed these last years like object kinetic Monte Carlo (OKMC) and phase-field (PF) models. Although hardly applicable for low sink volume fractions, OKMC turns out to be efficient in calculating the sink strength for 1D/3D migrating defects in a lot of cases [10,11]. PF methods have been applied to predict microstructure evolution under irradiation taking into account elasticity in presence of dislocation loops [12,13] acting as sinks. This approach is idoneous to tackle this type of problem since it can easily incorporate the microelasticity theory [14–17] associated to any dislocation network, and couple it to the diffusion of the migrating species. Although there is an increasing number of works concerning PF models of radiation damage, there is still no comprehensive comparison of the PF predicted values of the sink strength with data available in the literature. The reliability of PF models to quantitatively evaluate sink strength and consequently the growth rate of the sinks, with or without elasticity, is then still under debate.

The aim of this paper is twofold. Its first objective is to show that the PF methodology can be used to predict with an excellent accuracy the value of the sink strength in a number of test cases for which the sink strength is exactly known. The second objective is to calculate the sink strength of a dislocation taking into account elasticity without necessarily making the assumptions made so far and needed to obtain an analytical solution. Our results clearly show that existing values of sink strength for dislocations which interact with PDs through an elastic field are significantly underestimated. To expose these results, the article is organised as follows. Section 2 presents an original PF model to treat dislocations as a sink. Section 3 compares the numerical PF results with analytical solutions for some reference cases, which allows to conclude on the capabilities and limitations of the PF model to calculate dislocation sink strengths. Finally, we will show specific cases for which this PF model allows to calculate sink strength beyond the theoretical cases presented in the literature.

2. Methodology

2.1. System description: definition of the order parameters

The computational approach used in this paper rests on a PF model which is modified to take into account the creation of PDs by radiation and their absorption by localized sinks. We consider a single crystal with a PD site fraction field $X(\mathbf{r})$ interacting with dislocations which act as PD sinks. In this work, 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, which means that $X(\mathbf{r})$ refers either to vacancies or SIAs. Moreover, it is assumed that the chemical and elastic interactions between these two types of PDs have no influence on the resulting sink efficiencies. As a consequence, the definition of only one conserved order parameter field, corresponding to vacancy or SIA site fraction, is required in the simulations.

In order to calculate the sink efficiency of a dislocation, its stress field must be correctly simulated, since it strongly modifies the diffusion of the migrating species around it. This can be easily performed in PF models based on the equivalence demonstrated by Nabarro [18] that a platelet of thickness d characterised by a stress-free strain ϵ_{ij}^{d0} gives the same stress field as a dislocation loop embracing this platelet along its perimeter provided that:

$$\epsilon_{ij}^{d0} = \frac{1}{2d}(b_i n_j + b_j n_i), \tag{2}$$

with b_i and n_j respectively the ith component of the Burgers vector $\mathbf{b}$ and the jth component of the unit vector $\mathbf{n}$ normal to the habit plane of the loop. In PF models, d is usually replaced by the grid spacing a_0 in Eq. (2). Any type of dislocations can then be modelled by means of the order parameter $\eta(\mathbf{r})$ equal to 1 inside the platelet and 0 outside. If a dislocation loop is modelled, $\eta(\mathbf{r})$ increases sharply from 0 to 1 along the direction normal to its habit plane. Conversely, $\eta(\mathbf{r})$ gradually changes from 1 to 0 along a diffuse interface of width W and located at the dislocation core along a line crossing the loop and contained in its habit plane. W is typically of the order of 3–4 numerical cells in PF models.

Dislocation modelling in PF method is well-known, as mentioned in the introduction, but the correct modelling of the sink behaviour of a dislocation is still a challenge, even if an attempt towards this goal is proposed in [12,13]. In these works, interstitials loops are considered as platelet-like precipitates with a non physical composition of 100% of SIAs in order to simulate the growing of an extra atomic plane when the loop extends. This choice necessarily introduces artificial SIA compositions at the interfaces between the loop and the matrix, and this may in turn influence the SIA diffusion field around the dislocation and hence the calculated sink efficiency. In order to avoid this drawback, another method is presented in this work, which introduces an additional order parameter $\lambda(\mathbf{r})$ equal to 0 in the matrix and 1 in the capture zone of the sink. The composition in the sink is maintained at a constant value X^s by adding an absorption flux $J^{abs}(\mathbf{r})$ to the PD conservation equation as explained in Section 2.3.