# Numerical evaluation of dislocation loop sink strengths: A phase-field approach

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A B S T R A C T

A phase-field method is applied to compute the sink strength of dislocation loops in irradiated materials. This model enables to consider various sink geometries and long range elastic interactions between dislocation loops and migrating defects. Our results show that the analytical solutions underestimate the sink strength of loops. In addition, the influence of elasticity on sink strength increases with the loop radius. Finally, there is a significant effect of the dislocation line configuration enhanced by elasticity.

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## 1. Introduction

While dislocation loops are commonly observed defects in irradiated metals, their point defect (PD) sink strengths have been much less studied than straight dislocations, due to their 3D nature. In order to better understand microstructure evolution in irradiated metals, dislocation loops should benefit from the same efforts as those dedicated to straight dislocation lines.

Straight dislocations have been studied for more than 50 years. The first models described the dislocation as a cylindrical PD sink embedded in a sink-free volume of the same shape (the "hollow cylinder model"), which allowed to propose several analytical solutions, depending on boundary conditions (see [1] for a review): (i) the average PD concentration is maintained constant at the border of the sink-free volume (Laplace model), (ii) the PD flux at the border of the sink-free region is set at zero, PD creation by irradiation is modelled by a volumetric source term in the diffusion equation, and the sink strength is deduced from the outer border concentration (Poisson model), (iii) the same assumptions as in (ii) are used, but the average concentration in the sink-free volume is considered for the sink strength calculation, instead of the outer border concentration (Wiedersich model). In the models described by Nichols [1], the effect of the dislocation stress field on PD diffusion was neglected. As the elastic drift is thought to be one of the

driving forces for swelling in irradiated fcc crystals [2,3], the elastic interaction between the dislocation line and PDs has been first taken into account assuming that the crystal properties were isotropic with PDs modelled as dilatation centres [4–9]. More recent works considered the influence of the anisotropy of the crystal and of the PD shape in its equilibrium [10] and saddle point configuration [11–16] on sink strength. Most of those studies are limited to straight dislocations, which can be simulated in 2D, unlike dislocation loops. As a consequence, the calculation of the PD flux to the loops is much more challenging.

Seeger et al. [17] proposed a solution of the Laplace equation for the toroidal sink, isolated in an infinite medium. Jansson et al. [18] computed the sink strength of dislocation loops by means of an Object Kinetic Monte Carlo (OKMC) method [19]. This technique allows to simulate realistic irradiation conditions and to investigate the effect of diffusion anisotropy, but the elastic interactions were not considered in their work. Whereas the stress field generated by an isolated straight dislocation can be analytically obtained in some specific cases [20], the same work remains a tricky issue for dislocation loops. In most analytical works, a solution to this problem is proposed under the assumption that the loop is elastically equivalent to a spherical sink [21,22]. The true toroidal geometry of the loop has been numerically considered in the work of Dubinko et al. [8]. In particular, they showed 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.

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Most recent numerical techniques are still limited to simplifying assumptions (Laplace boundary conditions) or must be coupled with other models to provide the PD elastic potential around the dislocation. Rouchette et al. [9] developed a numerical phase-field (PF) method free of any topological limitations that enables to consider the migration of PDs in a dislocation network in realistic conditions. Their technique, based on the microelasticity theory [23–25], naturally takes into account the long range interaction between the microstructure and the migrating defects, provided that the following input parameters are known: the PD stress-free strain tensor (obtained by *ab initio* calculations), the Burgers vector and the vector normal to the habit plane of the dislocation.

While this method was first applied to straight dislocations [9,26], the goal of this paper is to show that the PF model can be easily generalised to complex microstructures, such as dislocation loops, to calculate sink strengths. The article is then organised as follows. Section 2 briefly recalls the PF methodology used to calculate sink strengths and a proper definition of the order parameters is proposed for the case of dislocation loops. The PF results presented in Section 3 allow to discuss the validity of the previous analytical models. Moreover, since the stress field is strongly dependent on the dislocation configuration (straight line *vs* loop), the elastic effect on sink strength is quantified in both cases and compared, a task that can be directly performed with the PF model.

## 2. Methodology

In this section, a brief summary of the main assumptions and basic methodological issues of the PF model are given. All the details can be found in [9]. The model solves the following kinetic equation in presence of dislocation lines that generate an elastic field and act as perfect sinks:

$$\frac{\partial X}{\partial t} = D\nabla^2 X + \frac{D}{k_B T}\mathbf{\nabla}\left[X\mathbf{\nabla}\mu_{el}\right] + K_0 - J^{abs} \tag{1}$$

with $X$ the PD site fraction, $D$ the diffusion coefficient (taken isotropic in this work), $\mu_{el}$ the elastic potential, $K_0$ the PD generation rate and $J^{abs}$ the PD absorption flux at the sink. Its expression is given by Eq. (6) and is justified below. In this paper, we extended the method in 3D in order to treat dislocation loops. In the following, we define the order parameters for that case, and recall their part in the model.

In Eq. (1), the calculation of the elastic potential $\mu_{el}$ is based on the microelasticity theory [23], which consists in associating to each defect the relevant eigenstrain or stress-free strain. By means of eigenstrains and order parameters, elastic interactions between defects are naturally taken into account whatever their morphological configuration. According to Nabarro [20], one dislocation loop is elastically equivalent to the platelet of thickness $a_0$ it encompasses and characterised by a stress-free strain $\epsilon_{ij}^{d0}$ defined as:

$$\epsilon_{ij}^{d0} = \frac{1}{2a_0}(b_i n_j + b_j n_i), \tag{2}$$

with $b_i$ and $n_j$ respectively the $i$th component of the Burgers vector **b** and the $j$th component of the unit vector **n** normal to the habit plane of the loop, and $a_0$ the cell size of the calculation domain. Owing to that equivalence, a loop is modelled by means of the order parameter $\eta(\mathbf{r})$ equal to 1 inside the platelet and 0 outside. In our case, a disc-shaped platelet of radius $r_L$ is considered, hence, the dislocation is a circular loop (see Fig. 1a). The local stress-free strain due to the loop is $\varepsilon_{ij}^d(\mathbf{r}) = \epsilon_{ij}^{d0}\eta(\mathbf{r})$.

The local stress-free strain due to the PD site fraction $X(\mathbf{r})$ is given by:

$$\varepsilon_{ij}^0(\mathbf{r}) = \epsilon_{ij}^{00}X(\mathbf{r}), \tag{3}$$
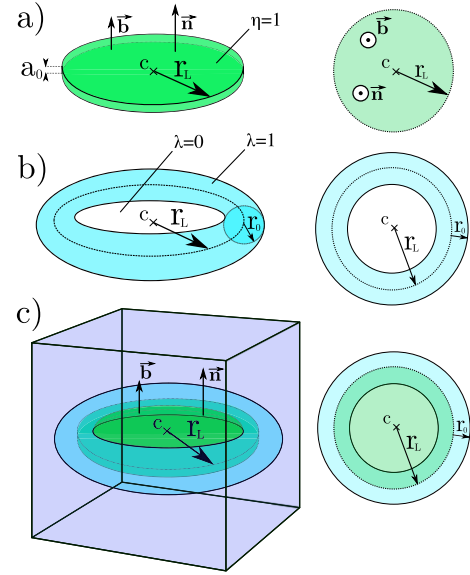


**Fig. 1.** (a) Definition of the platelet (with the same centre c as the torus) that represents the circular dislocation loop with thickness $a_0$ and radius $r_L$ by means of $\eta$. (b) Definition of the toroidal sink domain centred on $c$ with radius $r_L$ and core radius $r_0$ by means of $\lambda$. (c) Coexistence of both order parameters in the simulated system.

where $\epsilon_{ij}^{00}$ is the Vegard tensor. The relaxation volume $\Omega$ is related to the Vegard tensor through the relation $\text{Tr}(\epsilon^{00}) = \Omega/V_{at}$. The Vegard tensor can be determined as follows. If one PD is introduced in a supercell of the perfect crystal containing $N_{at}$ atomic sites, this supercell relaxes, which results in a homogeneous strain $\varepsilon_{ij}$. The Vegard coefficients are given by:

$$\epsilon_{ij}^{00} = N_{at}\varepsilon_{ij}. \tag{4}$$

If the supercell of volume $V_{sp}$ is not allowed to relax, the presence of one PD acts as a source of internal stress $\sigma_{ij}$ related to the elastic dipole tensor $P_{ij}$ through:

$$P_{ij} = V_{sp} \times \sigma_{ij}, \tag{5}$$

with $\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$, where $C_{ijkl}$ are the elastic constants of the matrix. It follows from Eqs. (4) and (5) that $P_{ij} = V_{at}C_{ijkl}\epsilon_{kl}^{00}$, with $V_{at}$ the atomic volume. Starting from the knowledge of **b**, **n**, $\epsilon^{00}$ and the elastic constants of the matrix $C_{ijkl}$, one can compute the elastic potential $\mu_{el}$ of the PD for any dislocation network.

In order to model the PD absorption at the dislocation core, the term $J^{abs}(\mathbf{r})$ in Eq. (1) is defined as:

$$J^{abs}(\mathbf{r}, t) = \lambda(\mathbf{r}) \cdot \lambda^{eff} \cdot [X(\mathbf{r}, t) - X^s] \tag{6}$$

Eq. (6) has been proposed in [27] to simulate PD absorption in restricted and locally well defined regions of the PF calculation domain. It introduces an additional order parameter $\lambda(\mathbf{r})$ equal to 0 in the matrix and 1 in the capture zone of the sink. For dislocation loops, the capture zone is supposed to be circular, of radius $r_0$ and located around the dislocation cores. Then, $\lambda$ is set at 1 in a torus with major radius $r_L$ and minor radius $r_0$ (see Fig. 1b). This last parameter corresponds to a new degree of freedom in the PF model. It allows a precise control of the sink geometry, which is essential to correctly calculate the sink strength. Eq. (6) ensures that $J^{abs}(\mathbf{r}, t)$ is zero in all the volume except inside the toroidal sink.

$X^s$ is the PD site fraction at the surface of the sink: it depends on the PD and the nature of the sink and is an input of the model. It is generally chosen as the PD thermal equilibrium composition ($= \exp(-E_f/k_B T)$, $E_f$ being the PD formation free energy). In this