



Mechanics of point defect diffusion near dislocations and grain boundaries: A chemomechanical framework

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ABSTRACT

Diffusion of point defects during irradiation is simulated via a two-way coupling between mechanical stress and defect diffusion in iron. This diffusion is based on a modified chemical potential that includes not only the local concentration of radiation-induced defects, but also the influence of the residual stress field from both the microstructure (i.e. dislocations or grain boundaries) and the eigenstrain caused by the defects themselves. Defect flux and concentration rates are derived from this chemical potential using Fick's first and second laws. Mean field rate theory is incorporated to model the annihilation of Frenkel pairs, and increased annihilation near grain boundaries is included based on the elastic energy of each grain boundary. Mechanical equilibrium is coupled with diffusion by computing eigenstrain from point defects and adding this to the total strain. Intrinsic stresses associated with the dislocations and grain boundaries are calculated using dislocation and disclination mechanics. Through this two-way-coupled model, regions of low concentration are seen near grain boundaries, and sink efficiency is calculated for different types of microstructure. The results show that the two-way mechanical coupling has a strong influence on sink efficiency for dislocation loops. The results also suggest that misorientation is a poor metric for determining sink efficiency, with sink density and elastic energy being much more informative.

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1. Introduction

The concentrations of self-interstitial atoms (SIAs) and vacancies are relatively low in metals at thermal equilibrium. Under irradiation, however, these point defects (PDs) begin to accumulate and, when temperatures are high enough to permit mobility, migrate toward PD sinks. Eventually this process reaches a new equilibrium where the implantation of defects is balanced by their removal at sinks and via SIA-vacancy recombination. These equilibrium concentrations are magnitudes larger than those observed in the absence of radiation. Over time, this increase in PDs can lead to an accumulation of damage and can cause radiation-induced segregation (RIS) to occur in alloys [1]. Understanding the interactions between PDs and sinks is critical in understanding how to mitigate the damage caused by irradiation [2].

Some microstructural features, such as dislocations, grain boundaries, and triple junctions, tend to attract PDs and act as sinks. For example, PDs are removed relatively quickly by the high density of interphase boundaries, grain boundaries, and pores in nanomaterials [2–4]. As such, the radiation tolerance of nano-grained metals is largely due to the high volume fraction of grain boundaries which reduces the overall concentration of PDs at equilibrium during irradiation. These materials benefit significantly from this effect, allowing them to resist the effects of radiation damage that are commonly seen in metals with larger microstructure [5,6]. This type of resistance has been observed for a number of material systems [3–5].

One possible mechanism of PD migration is through the interaction between defects and mechanical stress, which has been studied using several methods. One such approach by Li et al. [7] uses a thermodynamic framework to describe the chemical potential of defects dissolved in a solid. This was expanded [8,9] to describe interstitial hydrogen in iron and steel subjected to an externally-applied stress field. Later work by Larché and Cahn [10,11] builds

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upon this concept to describe solids subjected to multicomponent stresses, resulting in distinct chemical and elastic equations. Recently, Rouchette et al. [12] describe a phase field model in which stress gradients around certain defect sinks introduce a diffusion drift. In all of these cases, the diffusion of defects is shown to not only depend on local concentration gradients, but also on compositional strain arising from material geometry and long-distance compositional inhomogeneities [13,14]. Swaminathan et al. [15] have derived a generalized chemical potential for solutes in solids that includes a term for mechanical effects. More recently, Cui et al. [16] derive the expression for this mechanical term based on the strain energy of a solute in the solid matrix.

Regardless of the method used, modeling PD diffusion remains difficult due to the complexity of the materials involved, with multiple phases, alloying elements, and defects all playing significant roles in more complex systems. Atomistic models are useful for capturing a wide range of these effects, but they are ill-suited for large time and length scales. Mesoscale models, such as mean field rate theory, are more suited to larger time and length scales, but they often lack a full description of the coupling between mechanical stress and diffusion rates. Continuum models can be used for larger scales, but they require a number of input parameters that are drawn from atomistic results and first principle calculations. For this reason, PD diffusion and RIS are multi-scale problems where simulations must combine techniques ranging from atomistic to continuum scales [1].

The present work focuses on the primary damage processes near dislocations and grain boundaries. The approach used combines all three of these scales in order to model PD diffusion near various microstructural sinks. Diffusion and mechanical equilibrium are calculated using a continuum approach based on a central finite difference scheme and small-strain finite element method, respectively. Point defect annihilation is modeled using an approach based on mean field rate theory, where homogeneity is assumed within each element and concentrations are handled using mean values; individual defects are not explicitly modeled. Atomistic effects are incorporated via the use of binding energy, migration energy, compositional expansion coefficients, and other parameters that influence both the diffusion and mechanical equations.

PD sinks are represented in two ways in the present model. Primarily, they are regions in which diffusing defects are removed via absorption. In addition, they are also represented by their intrinsic stress fields. This combined approach is comparable to the phase field approach used by Rouchette et al. [12] to describe point defect sinks. The stresses associated with an edge dislocation are represented using the classical continuum formulation, and low-angle symmetric tilt grain boundaries can be represented using repeating edge dislocations [17]. For the present work, disclination dipoles are used to construct tilt boundaries (via the Disclination Structural Unit Model or DSUM [18–20]) for a wide range of tilt angles. This avoids the limitation of the dislocation model, which is limited to low-angle boundaries. The resulting segregation profiles at equilibrium are analyzed to determine the efficiency of different point defect sinks and the suitability of this method for modeling PD diffusion under irradiation.

The subsequent sections are organized as follows. Section 2 gives the modified chemical potential upon which this formulation is based, derives the diffusion and mechanical equilibrium equations, describes additional rates and assumptions, and give expressions for intrinsic stress fields around line defects and grain boundaries. Section 3 presents simulation results and notable observations obtained using this formulation. Section 4 draws conclusions regarding the fitness of this model for describing defect interactions and segregation.

2. Micromechanical model of irradiation-induced point defect diffusion to microstructural defects

The present model features two-way coupling between defect diffusion and mechanical stress. On one hand, diffusion is based on a modified chemical potential that includes not only local concentration, but also hydrostatic stress. Defect flux and concentration rates are derived from this chemical potential using Fick's first and second laws. On the other hand, mechanical equilibrium is coupled with diffusion by accounting for eigenstrain due to the presence of point defects. As a result, defects tend to diffuse in response to the applied stress field, and the stresses are relieved over time as defects approach their preferred distribution and relax the microstructure.

2.1. Stress-dependent defect migration

Migration of vacancies and self-interstitial atoms (SIAs) is based on Fickian diffusion using a modified diffusion potential μ_α . The subscript α indicates the defect species, I for SIAs and V for vacancies. Per Fick's first law, the defect flux \mathbf{J}_α of species α is calculated from the gradient of the diffusion potential:

$$\mathbf{J}_\alpha = -\frac{D_\alpha c_\alpha}{RT} \nabla \mu_\alpha, \quad (1)$$

where D_α is diffusivity, c_α is defect concentration, R is the standard gas constant, and T is absolute temperature. The rate of concentration change is based on Fick's second law:

$$\frac{\partial c_\alpha}{\partial t} = -\nabla \cdot \mathbf{J}_\alpha + \sum_\beta a_{\alpha\beta} f_\beta, \quad (2)$$

where the additional $a_{\alpha\beta} f_\beta$ terms in Eq. (2) are used to account for SIA-vacancy annihilation and defect implantation. Calculation of the rates f_β is described in Section 2.2. Selection of the coefficients $a_{\alpha\beta}$ depends upon the nature of rate f_β and the type of defect α . For example, if the rate f_β describes mobile vacancies and SIAs annihilating, and α represents vacancies, then $a_{\alpha\beta} = -1$. This is due to the fact that each annihilation event removes a single vacancy.

The modified diffusion potential is given by [15]:

$$\mu_\alpha(c_\alpha, t) = \mu_\alpha^{(0)} + RT \ln(\gamma_\alpha c_\alpha) - V_m \eta_\alpha \sigma_{kk}, \quad (3)$$

where $\mu_\alpha^{(0)}$ is the diffusion potential at a standard state, γ_α is the activity coefficient, V_m is the molar volume of the pure solid, η_α is the coefficient of compositional expansion (CCE), and σ_{kk} is the trace of the Cauchy stress tensor. The last term in the right-hand side of Eq. (3) represents the coupling of diffusion with mechanical stress. Combining Eqs. (1)–(3), the rate of change for defect concentration is expanded as:

$$\frac{\partial c_\alpha}{\partial t} = D_\alpha \left[\left(1 + \frac{c_\alpha}{\gamma_\alpha} \frac{\partial \gamma_\alpha}{\partial c_\alpha} \right) \nabla^2 c_\alpha + \nabla \cdot \left(\frac{c_\alpha}{\gamma_\alpha} \frac{\partial \gamma_\alpha}{\partial c_\alpha} \right) \cdot \nabla c_\alpha - \frac{V_m \eta_\alpha}{RT} \left(\nabla c_\alpha \cdot \nabla \sigma_{kk} + c_\alpha \nabla^2 \sigma_{kk} \right) \right] + \sum_\beta a_{\alpha\beta} f_\beta. \quad (4)$$

It follows the form derived by Cui et al. [16] with one additional assumption: the elastic response is assumed to be independent of the concentration of defects,

$$\frac{\partial \mathbf{C}}{\partial c_\alpha} \approx 0, \quad (5)$$

and the activity coefficient γ_α is given by Eq. (6):

$$\gamma_\alpha = \frac{1}{1 - c_\alpha}. \quad (6)$$

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