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A continuous model including elastodiffusion for sink strength calculation of interfaces

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ABSTRACT

Object kinetic Monte Carlo and finite-element calculations have been used to calculate the sink strength of low-angle symmetric tilt grain boundaries (STGBs) in Cu. It is shown that saddle point anisotropy of vacancies increases their absorption by STGBs, making these interfaces nearly neutral sinks. The continuous model, which includes point defect anisotropy at saddle point, is able to reproduce OKMC calculations, provided the exact value of the diffusion tensor is retained. The use of elastodiffusion tensor is not valid, due to the large strains ($\varepsilon \sim 10^{-2}$) created by STGBs. The low numerical cost of the continuous model could allow for a more systematic investigation of radiation tolerance due to interfaces.

1. Introduction

In inhomogeneous materials subjected to irradiation, interphase and grain boundaries between crystalline solids are known to be sinks for point defects such as vacancies and self-interstitial atoms (SIAs). The diffusion and absorption of supersaturated point defects at interfaces can alter their structure, for example contributing to void growth [1] and solute enrichment or depletion [2]. Such evolutions at interfaces can degrade the mechanical properties of materials [3] and accelerate the failure under irradiation. Conversely, it has been observed that the presence of a high density of interfaces could reduce the radiation induced damage in the matrix [4,5]. The ability of interfaces to remove point defects from the matrix is rationalized in terms of "sink efficiency" [6]. It has been shown that the sink efficiency depends on the interface type [7], thus on the interface structure and energy. For grain boundaries, different sink efficiencies have been inferred for different misorientations, based on the width of void-denuded zones [8]. Nanostructured materials with "super-sink" interfaces may therefore be optimally designed in order to dramatically enhance radiation tolerance [9].

Sink efficiencies depend on how defects interact with the interface when they reach it [10,11]. Usually, to determine sink efficiencies it is assumed that defects perform a random walk in the matrix [12,7]. However, the elastic interaction between the interface and defects can bias the atomic jumps and increase the flux of defects. Such elastic effects can be quantified by the "sink strength" of the interface for a given type of defect. Sink strengths of low-angle grain boundaries have been calculated by King and Smith [13], and more recently by Jiang et al. [14]. In these works, point defects were considered as isotropic elastic inclusions. This approximation permits to reduce the sink strength calculation to the solving of a single partial differential equation (PDE) on the defect concentration. To account for the different interstitial and vacancy configurations at stable and saddle points, an object kinetic Monte Carlo (OKMC) was used [15]. In this study it was shown that the anisotropy of point defects at their saddle point, which contributes to elastodiffusion [16], is responsible for a significant enhancement of the sink strength. OKMC simulations, however, are somewhat less efficient than the low-cost and practical finite difference or finite-element method (FEM) solving of PDEs. These methods could also be preferable for rapidly scanning over many different interfaces in computational strategies for tailoring composite materials.

In order to systematize the calculation of sink strength of interfaces, an important question is to know whether a continuous model can achieve the same level of accuracy as OKMC. We will prove that this is indeed the case, provided the local diffusion tensor under stress is not approximated by using the elastodiffusion tensor. The validity and the accuracy of the continuous approach are shown in the case of low-angle symmetric tilt grain boundaries (STGBs) in Cu.

2. Methods for sink strength calculations

Low-angle STGBs in Cu with various misorientations θ are studied.

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We suppose that values of θ are low enough to consider that defects can only be absorbed at the discrete dislocations [12]. Elastic fields created by such interfaces are generated using either isotropic or anisotropic elasticity. For isotropic elasticity, a closed form expression for the displacement and distortion fields exists [17]. Such an expression cannot (in general) be explicitly written for general anisotropic elastic cases. In the present work, the complete interface strain fields are determined by combining and solving the quantized Frank-Bilby equation with anisotropic elasticity theory [18], consistently with the misorientation and interface plane orientation and with vanishing far-field stresses. The interfacial dislocation-based method has been successfully validated through comparisons with experiments for [0 0 1] tilt boundaries [18] and with atomistic simulations for heterophase interfaces [19].

The interaction energy between a point defect and a dislocation-induced strain field ε_{ij} reads [20,21]

$$E^{\mathrm{e/s},k}(\boldsymbol{r}) = -\sum_{i,j} P_{ij}^{\mathrm{e/s},k}\varepsilon_{ij}(\boldsymbol{r}), \tag{1}$$

where $P_{ij}^{\mathrm{e/s},k}$ is the elastic dipole tensor for defect configuration k. For example, it can be [1 0 0], [0 1 0] or [0 0 1] for an SIA at its stable position. Superscripts 'e' or 's' indicate whether the dipole tensor corresponds to a stable (equilibrium) or saddle position, respectively. Elastic dipole tensors were obtained previously by first principles calculations for SIAs and vacancies in Cu at both stable and saddle positions [15].

To calculate the sink strengths of interfaces, two different methods are used and compared. The first one is an OKMC approach [15,22], which can naturally handle various defect configurations, both at stable and saddle positions. It accounts for the atomistic details of migration. Since defects are not allowed to reorient on their site in our simulations, in agreement with experimental observations [23] and numerical calculations [24], we take into account the fact that a given defect configuration will only be coupled to three migration channels (out of four) with specific configurations [25]. OKMC will be used to produce reference results.

The second method relies on the FEM solving of a PDE on a variable linked to the concentration field, which is viewed as a significant simplification of a complex diffusion problem and also provides an opportunity for rigorous validation with the first resource-intensive calculations. The continuous model of transport relates the local flux of defects to the concentration gradient. Due to the existence of three stable configurations for SIAs, in principle three different and coupled concentration fields must be followed. However, as noted in Refs. [26,16], it is reasonable to suppose that thermal equilibrium for the different configurations is quickly achieved. In the present study, equilibrium cannot come from an on-site reorientation, which is not enabled in the present OKMC model. Instead it should be a consequence of the migration of defects and of the detailed balance. The assumption of thermal equilibrium can be checked in OKMC simulations. It was shown that if this condition if fulfilled, the flux can be simply written as [16]

$$\boldsymbol{J}(\boldsymbol{r}) = -\widetilde{\boldsymbol{D}}(\boldsymbol{r})\nabla u(\boldsymbol{r}), \tag{2}$$

where $u(\boldsymbol{r}) = \sum_{k=1}^{s} u^k(\boldsymbol{r})$ at position $\boldsymbol{r}$, and the renormalized concentration of configuration k ($k = 1, ..., s$) is given by

$$u^k(\boldsymbol{r}) = c^k(\boldsymbol{r})\exp(\beta E^{\mathrm{e},k}(\boldsymbol{r})). \tag{3}$$

Here $c^k(\boldsymbol{r})$ is the concentration of configuration k and $\beta = 1/k_{\mathrm{B}}T$, with k_{B} the Boltzmann constant and T the temperature. Because the thermal equilibrium between all configurations is assumed, for two specific and distinct configurations k and l we have $c^k(\boldsymbol{r})/c^l(\boldsymbol{r}) = \exp(-\beta E^{\mathrm{e},k}(\boldsymbol{r}))/\exp(-\beta E^{\mathrm{e},l}(\boldsymbol{r}))$ and u^k is independent of k. The concentration of each configuration is thus related to u through

$$c^k(\boldsymbol{r}) = \frac{1}{s}u(\boldsymbol{r})\exp(-\beta E^{\mathrm{e},k}(\boldsymbol{r})). \tag{4}$$

The renormalized diffusion tensor is given by [16]

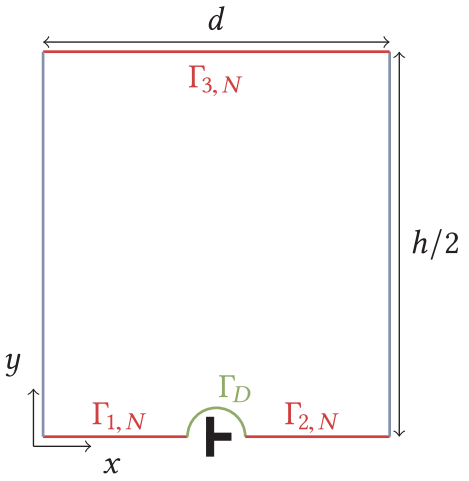

Fig. 1. Decomposition of the computational domain boundaries to compute the sink strength of a low-angle STGB (see text for details).

$$\widetilde{D}_{ij}(\boldsymbol{r}) = \frac{1}{2}\nu\kappa\sum_{\boldsymbol{h}} h_i h_j \exp(-\beta E^{\mathrm{s},\boldsymbol{h}}(\boldsymbol{r})). \tag{5}$$

The summation is on the different possible jumps $\boldsymbol{h}$. In the present analysis, we have used $E^{\mathrm{s},\boldsymbol{h}}$ instead of $E^{\mathrm{s},k}$ to identify the interaction energy of the defect at saddle point for a particular jump $\boldsymbol{h}$, since only one saddle configuration is associated to a given jump. In Eq. (5) the jump frequency without any elastic interactions is $\nu = \nu_0\exp(-\beta E^{\mathrm{m}})$, with E^{m} the migration energy and ν_0 the attempt frequency, which does not depend on the jump $\boldsymbol{h}$. Factor κ is equal to 1 for vacancies and 2/3 for $\langle 1\,0\,0\rangle$-split dumbbells SIAs.

At stationary state, the continuity equation on the total renormalized concentration of defects reads

$$G - \nabla\cdot\boldsymbol{J} = 0, \tag{6}$$

where G is the creation rate and $\boldsymbol{J}$ is defined by Eq. (2).

This equation is solved for the two-dimensional system shown in Fig. 1. Sinks are cylinders of radius $r_c = 2b$ centered at dislocations, where b is the Burgers vector ($b = 0.362$ nm). Two grain boundaries are separated by $h = 70$ nm, so that elastic fields produced by each grain boundary do not overlap for all values of θ considered. The distance d between dislocations along the GB is related to θ through $d = b/(2\sin(\theta/2))$. Boundary conditions are

$$u(\boldsymbol{r}) = 0 \quad \forall\, \boldsymbol{r} \in \Gamma_D \tag{7}$$

$$u(d, y) = u(0, y) \tag{8}$$

$$\widetilde{\boldsymbol{D}}\nabla u\cdot \mathrm{d}\boldsymbol{S} = 0 \quad \text{on} \quad \Gamma_{i,N}(i = 1, 2, 3). \tag{9}$$

We have assumed that the system can be considered as a two-dimensional system, *ie* with only flux components along x and y. Even for a system which is structurally invariant along one direction, fluxes can appear in the direction of invariance (although the total flux is zero), due to the anisotropy of defects at their saddle position [22]. We now justify this hypothesis.

If present, such fluxes are due to cross-terms $\widetilde{D}_{31}$ and $\widetilde{D}_{32}$ which couple $\partial u/\partial x$ and $\partial u/\partial y$ to J_z. It is straightforward to check that terms which contribute to $\widetilde{D}_{31}$ and $\widetilde{D}_{32}$ in Eq. (5) are not zero. However, for a given jump $\boldsymbol{h} = (h_1, h_2, h_3)$ with an elastic dipole (in Voigt notation) $\boldsymbol{P} = (P_{11}, P_{22}, P_{33}, P_{23}, P_{31}, P_{12})$, there exists a jump $\boldsymbol{h}' = (h_1, h_2, -h_3)$ with an associated elastic dipole $\boldsymbol{P}' = (P_{11}, P_{22}, P_{33}, -P_{23}, -P_{31}, P_{12})$. Therefore, owing to Eq. (1) the defect has the same saddle point energy for the two jumps if $\varepsilon_{23} = \varepsilon_{31} = 0$, which is precisely the case in the present low-angle STGBs. Contributions to $\widetilde{D}_{31}$ and $\widetilde{D}_{32}$ cancel each other out, so that $\widetilde{D}_{31} = \widetilde{D}_{32} = 0$ and J_z is zero.

The problem given by Eqs. (2) and (6) with Eqs. (7)–(9) can be