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Self-healing of low angle grain boundaries by vacancy diffusion and dislocation climb

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ABSTRACT

A new analytical model was developed to quantify the role of dislocation climb assisted by vacancy pipe and bulk diffusion in controlling the damage resistance and self-healing of perturbed low angle grain boundaries. Dislocation climb assisted by vacancy pipe diffusion predominantly controls the self-healing process at lower temperatures, while that assisted by bulk diffusion becomes important only at higher temperatures. A relaxation time for the perturbed grain boundary structure was also derived to quantify the time associated with the self-healing process. The extent of this self-healing increases with decreasing grain size, which explains the enhanced damage resistance of nanocrystalline materials.

Extending the lifetime of materials is one of the ultimate goals of material design and development. Major challenges to achieving this goal include improving damage resistance and the ability of a material to recover from damage (i.e., self-healing). Experimental observations indicate that grain boundaries (GBs) are potent sinks for many types of defects and, thus, may improve damage resistance [1–3]. A number of mechanisms have been proposed to explain the relationship between GB structure and its role as a defect sink [4–6]. However, GB self-healing remains poorly understood. In particular, an equilibrium GB structure can be disrupted by plastic deformation [7,8] (including severe plastic deformation (SPD) [9]) and radiation-induced damage [4] leading to non-equilibrium GB structures. The following question naturally arises: "what controls GB self-healing that leads to the relaxation of the GB to its equilibrium state?".

Given that GBs are neither ideal sinks or sources for point defects [3,10–12], dislocation climb assisted by diffusion [13–18] becomes an important factor in GB self-healing. Accordingly, in this letter, we examine the time scale over which a low angle tilt GB relaxes to its equilibrium structure and the role of coupled point defect transport and dislocation climb in this relaxation. It should be noted that the scenarios considered here follow those in [19]. The model presented here extends the earlier work by directly incorporating the effects of pipe diffusion-assisted dislocation climb (in addition to bulk diffusion, considered previously). In some circumstances, the inclusion of pipe diffusion leads to profound changes. This allows for a more accurate quantification of the damage resistance and self-healing properties associated with perturbed grain boundaries.

Here, we model a low angle symmetric tilt GB as a regular array of edge dislocations [20,21] as shown in Fig. 1(a), where the constituent dislocation lines are labeled γ_j ($j = \cdots, -2, -1, 0, 1, 2, \cdots$). For a perfect GB, each constituent dislocation has a line direction $\boldsymbol{\xi} = (0, 0, 1)$ and Burgers vector $\mathbf{b} = (b, 0, 0)$. The spacing between neighboring dislocations D is determined from the misorientation angle $\theta = b/D$. We describe damage in terms of a perturbation to this ideal, equilibrium GB structure. This is modeled here as a perturbation to the GB constituent dislocation profiles of amplitude ε, wavenumber k_3 along the dislocation, and phase shift k_2, as indicated in Fig. 1(b). Accordingly, the perturbation wavelengths in the y- and z-directions are $\lambda_2 = 2\pi/k_2$ and $\lambda_3 = 2\pi/k_3$, respectively. For $k_2 = 0$ case, λ_2 is any positive integral multiple of D, while for $k_3 = 0$, λ_3 is any positive number. The perturbation amplitude is positively correlated with the strength of the damage according to the energy-amplitude relationship (i.e., the energy transported by a wave is proportional to the square of its amplitude). On the other hand, the perturbation

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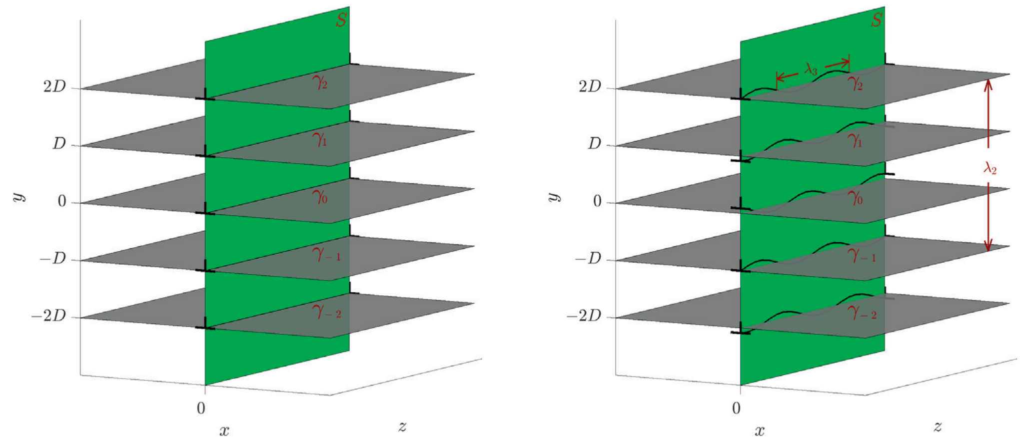

(a) (b)

Fig. 1. (a) Schematic representation of a low angle symmetric tilt grain boundary S consisting of a regular array of edge dislocations, γ_j ($j = \cdots, -2, -1, 0, 1, 2, \cdots$), with a regular spacing D. (b) Schematic representation of the perturbed constituent dislocations in the GB plane with a perturbation phase shift wavelength λ_2 in the y-direction and wavelength λ_3 along the dislocation line.

wavelength are correlated with grain size; larger grains can accommodate perturbations to the dislocation profiles of larger wavelength (see the online Supplementary material for details).

For a perturbed low angle tilt GB, climb of the constituent dislocations, enabled by point defect transport (we focus on the case of vacancies here), can lead to GB structure relaxation. The climb force $\mathbf{f}_{\rm cl}$ and climb velocity $\mathbf{v}_{\rm cl}$ are in the climb direction (i.e., in the direction $\boldsymbol{\xi} \times \mathbf{b}$) and their scalar forms are $f_{\rm cl} = \mathbf{f}_{PK} \cdot (\boldsymbol{\xi} \times \mathbf{b}/b)$ and $v_{\rm cl} = \mathbf{v} \cdot (\boldsymbol{\xi} \times \mathbf{b}/b)$, respectively, where, $\mathbf{f}_{PK} = (\boldsymbol{\sigma} \cdot \mathbf{b}) \times \boldsymbol{\xi}$ is the Peach-Koehler force and $\mathbf{v}$ is the dislocation velocity. A point on the jth perturbed dislocation $(0, y(z), z)$ and its climb velocity $v_{\rm cl}$ can be expressed as

$$y(z) = jD + \varepsilon e^{\omega t} \cos(2\pi j/N + k_3 z), \tag{1}$$

$$v_{\rm cl}(z) = \frac{\partial y(z)}{\partial t} = \omega \varepsilon e^{\omega t} \cos(2\pi j/N + k_3 z), \tag{2}$$

where ω is the perturbation growth rate. Note that for a small perturbation amplitude ε, $\mathbf{v}_{\rm cl}$ is, to leading order, in the y-direction since the climb direction is $\boldsymbol{\xi} \times \mathbf{b}/b \approx (0, 1, 0)$. This also applies to $\mathbf{f}_{\rm cl}$.

Using the superposition principle, $\mathbf{v}_{\rm cl}$ can be decomposed into two components: $\mathbf{v}_{\rm cl}^p$ assisted by vacancy pipe diffusion (i.e., diffusion along the dislocation core); and $\mathbf{v}_{\rm cl}^b$ assisted by bulk diffusion (diffusion in the crystal lattice, away from the dislocation core), such that [18]

$$\mathbf{v}_{\rm cl} = \mathbf{v}_{\rm cl}^p + \mathbf{v}_{\rm cl}^b. \tag{3}$$

The magnitudes of these individual velocities are

$$v_{\rm cl}^p = \mathbf{v}_{\rm cl}^p \cdot (\boldsymbol{\xi} \times \mathbf{b}/b) = D_v^p b \frac{{\rm d}^2 c_d^p}{{\rm d}s^2}, \tag{4}$$

$$v_{\rm cl}^b = \mathbf{v}_{\rm cl}^b \cdot (\boldsymbol{\xi} \times \mathbf{b}/b) = \frac{2\pi r_d D_v^b}{b^2 l_\phi} \left(\frac{1}{2\pi r_d} \int_{r=r_d} c \cdot {\rm d}l - c_d^b \right), \tag{5}$$

where r_d is the dislocation core radius (the core is assumed to be a uniform cylindrical tube centered on the dislocation line), D_v^p and D_v^b are the pipe and bulk diffusion coefficients, respectively. $l_\phi = \exp\left(-\Delta E^{bp}/k_B T\right)$ is the probability of vacancies hopping to the core from the bulk which is correlated with the difference between the energy barrier for vacancies hopping into the dislocation core from the bulk and that for vacancy diffusion within the bulk, ΔE^{bp}. In the limit that $l_\phi \to 0$ (i.e., $\Delta E^{bp} \gg k_B T$), the constituent GB dislocations act as perfect defect sinks/sources, where the vacancy concentration at the surface of the dislocation core is identical to the equilibrium vacancy concentration. For small or moderate ΔE^{bp}, dislocations are imperfect defect sinks/sources. We approximate the variation of the vacancy concentration around each dislocation as axisymmetric, relative to the local dislocation line such that $c(s)$ is the vacancy concentration in the bulk, where s is the arclength along the dislocation line. The equilibrium vacancy concentrations on the inside and outside of the dislocation core are $c_d^p(s) = c_0^p \exp\left(-f_{\rm cl}(s)\Omega/bk_B T\right)$ and $c_d^b(s) = c_0^b \exp\left(-f_{\rm cl}(s)\Omega/bk_B T\right)$, where Ω is the atomic volume, and c_0^p and c_0^b are the reference vacancy concentrations in the dislocation core and bulk.

Since dislocation climb is slow relative to vacancy bulk diffusion [20], we compute the vacancy concentration in the bulk assuming diffusion equilibrium [18],

$$\begin{cases} D_v^b \nabla^2 c = 0, \\ -\left.\frac{\partial c}{\partial n}\right|_{r=r_d} = \frac{1}{l_\phi} \left.\left(c - c_d^b \right)\right|_{r=r_d}, \\ c = c_\infty|_{|x|=\infty}, \end{cases} \tag{6}$$

where $\partial/\partial n$ is the spatial derivative in the direction of the outward normal to the local cylindrical core and c_∞ is a constant, far-field vacancy concentration. When $l_\phi \to 0$, Eq. (6) reduces to a Dirichlet boundary condition [18]. Elastic interactions between dislocations and vacancies may reduce the vacancy migration barrier and increase the drift of vacancies towards interfaces [22]. These effects are not considered here for the sake of simplicity. Accordingly, one should view the current model as a lower bound estimate of the effect of vacancy pipe diffusion. If the material has a net supersaturation of vacancies (e.g., under some irradiation conditions), there will be an additional uniform dislocation drift velocity [12,19]. Here we set $c_\infty = c_0^b$ to focus on the relaxation of the perturbed GB structure.

The perturbation growth rate ω can be decomposed into contributions from pipe and bulk diffusion

$$\omega = \omega^p + \omega^b, \tag{7}$$