Scripta Materialia 114 (2016) 35–40

Contents lists available at ScienceDirect

Scripta Materialia

journal homepage: www.elsevier.com/locate/scriptamat

Regular Article

Relaxation of low-angle grain boundary structure by climb of the constituent dislocations

Yejun Gu [a,b], Yang Xiang [c,*], David J. Srolovitz [b,d]

[a] Nano Science and Technology Program, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong
[b] Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA 19104, USA
[c] Department of Mathematics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong
[d] Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA 19104, USA

ARTICLE INFO

Article history:
Received 2 September 2015
Received in revised form 11 November 2015
Accepted 12 November 2015
Available online 17 December 2015

Keywords:
Grain boundaries
Dislocation dynamics
Dislocation climb
Grain boundary structure

ABSTRACT

We study the relaxation of perturbed low-angle tilt grain boundaries by climb of the constituent dislocations. Under the combined influence of the long-range effects due the Peach–Koehler force and vacancy diffusion, dislocation climb always stabilizes the grain boundaries on a time scale that is proportional to the square of the perturbation length scale and inversely proportional to the point defect diffusivity. This relaxation has a different nature from that of perturbed low-angle grain boundaries by dislocation glide, in which only the long-range Peach–Koehler force is important, leading to a perturbation relaxation time linearly proportional to the perturbation wavelength itself.

1. Introduction

Grain boundaries in polycrystalline materials have received considerable attention due to their important roles in determining a wide range of properties, e.g., in diffusivity and electrical resistivity, creep rate, and fracture stress [1,2]. The structure of grain boundaries strongly influences grain boundary properties, and many attempts have been made to understand the correlations between these. In the classical dislocation model of grain boundaries developed by Read and Shockley [3], low-angle grain boundaries consist of regular arrays of dislocations. When grain boundaries absorb, transmit, or emit lattice dislocations, for example during recrystallization or when dislocation plasticity is operating with the grains, the dislocation structure of the grain boundary is perturbed, modifying grain boundary properties. That is, the periodicity of the array of dislocations that makes up the grain boundary is destroyed. This inevitably raises the energy of the grain boundary as well as modifies its properties [4]. The question naturally arises, "what is the time scale over which the perturbed dislocation structure relaxes back to its equilibrium distribution?" In this paper, we examine this question in the discrete dislocation framework and perturbation (or stability) theory.

For slightly perturbed low-angle tilt boundaries, the well-known capillary force is proportional to the local grain boundary curvature; this stabilizes flat grain boundaries [5,6]. Rottman [7] examined the stability of symmetric, low-angle tilt grain boundaries with respect to effects of thermal fluctuations. Nazarov et al. [8] used Monte Carlo techniques to analyze the grain boundary structure change caused by the absorption of grain boundary dislocations. Zhu and Xiang [9] studied the glide force on the constituent dislocations of perturbed symmetric low-angle tilt boundaries. They showed that the stabilizing force comes from both the long-range interaction of the constituent dislocations and the local dislocation line tension effect, and derived a continuum model for this glide force.

At high temperature, dislocation climb plays an important role in both the plastic deformation and recrystallization of polycrystalline materials [1,2,10,11]. The role of climb of the constituent dislocations along grain boundaries was examined by Burton [12] and Balluffi et al. [13]. Li [14] examined the relationship between dislocation climb in grain boundaries and grain rotation. Lim et al. [15,16] studied the mobility of the low-angle grain boundary and its constituent dislocation structure through three-dimensional dislocation dynamics techniques. Winning et al. [17] incorporated the effect of dislocation climb on the rate of low-angle tilt boundary migration into the grain boundary mobility law. Liu et al. [18,19,20] studied dislocation interactions with low-angle grain boundaries using dislocation dynamics simulations incorporating dislocation climb velocity in the dislocation mobility law.

It is widely accepted that the dislocation climb takes places with the assistance of the vacancy/interstitial diffusion, and most of the available discrete dislocation dynamics simulations incorporating such dislocation climb mechanism consider vacancy/interstitial diffusions in the bulk [21,22]. Recently, Gu et al. [23] derived a general dislocation climb

* Corresponding author.
E-mail address: maxiang@ust.hk (Y. Xiang).

http://dx.doi.org/10.1016/j.scriptamat.2015.11.016
1359-6462/

formulation for arbitrarily curved dislocations in three-dimensions, which accounts for the long-range interaction of dislocations and vacancy/interstitial diffusion in the bulk. This new formulation gives an accurate solution to the classical vacancy/interstitial-assisted dislocation climb model [1], based on a Green's function solution for the point defect distribution. In this formulation, the dislocation climb velocity is determined by solving integral equations along the dislocations that incorporates the point defect distribution, the relationship between dislocation climb and point defect adsorption/emission and the climb component of the Peach–Koehler force; the result effectively replaces the classical climb rate/Peach–Koehler climb force proportionality that has been widely applied in dislocation dynamics simulations (akin to the glide mobility law where the dislocation glide velocity is proportional to the Peach–Koehler glide force) [1,24,25,26,21,22]. It has been shown [23] that the previously widely used local mobility law for climb is applicable in only a very limited set of circumstances.

In this paper, we employ our recently developed Green's function formulation [23] to study the stability of low-angle grain boundaries by climb of the constituent dislocations, with emphasis on the contribution of the long-range interaction of dislocations through vacancy/interstitial diffusion to dislocation climb. With inclusion of this new effect, we show that dislocation climb has a fundamentally different effect on the stability of low-angle grain boundaries than has been discussed in the literature [7,9].

2. Methodology

We focus on the classical case of low-angle symmetric tilt boundaries. In the classical dislocation model of grain boundaries [1,3], a low-angle symmetric tilt grain boundary consists of a regular array of edge dislocations $\gamma_j, j=\cdots,-2,-1,0,1,2,\cdots$, see Fig. 1(a). The distance between neighboring dislocations D is determined by the rotation angle θ and the magnitude of the Burgers vector $b=|\boldsymbol{b}|$ by $\theta=b/D$. We choose a coordinate system in which the tilt boundary is located at $x=0$, the constituent dislocations have line direction $\boldsymbol{\xi}=(0,0,1)$, and the Burgers vector is $\boldsymbol{b}=(b,0,0)$. We consider the stability of the tilt boundary subject to small perturbations in the shape of the constituent dislocations within the grain boundary plane, i.e., in the y direction, see Fig. 1(b). In this case, the perturbed constituent dislocations will also move within the grain boundary plane by climb.

The classical model for vacancy assisted dislocation climb, under the assumption that the vacancy distribution is determined such that the divergence of the vacancy diffusional flux is zero (equilibrium distribution), can be written as [1,23]

$$D_v \Delta c = b v_{cl}\, \delta(\Gamma), \tag{1}$$

$$c(r=r_d,t) = c_0 e^{-\frac{f_{cl}\Omega}{b k_B T}}, \tag{2}$$

$$c(|x|=\infty,t) = c_\infty, \tag{3}$$

where c is the vacancy concentration, v_{cl} is the dislocation climb velocity, f_{cl} is the climb component of the Peach–Koehler force, Γ refers to the positions of all dislocations in the entire system, $\delta(\Gamma)$ is the Dirac delta function of Γ, D_v is the vacancy diffusion coefficient, r is the distance to any point on the dislocations, r_d is the dislocation core radius, c_0 is a constant reference vacancy concentration, c_∞ is some constant vacancy concentration at infinity, Ω is the atomic volume, k_B is the Boltzmann constant, and T is the temperature. In the case considered here, all of the dislocations are pure edges.

The Green's function formulation in [23] reduces the above boundary value problem to the following integral equations from which the climb velocity v_{cl} can be solved. For any point (x,y,z) on the dislocations,

$$b\int_{\Gamma} G(x_d,y_d,z_d;x_1,y_1,z_1)\, v_{cl}(x_1,y_1,z_1)\, dl = c_0 e^{-\frac{f_{cl}(x,y,z)\Omega}{b k_B T}} - c_\infty, \tag{4}$$

where (x_d,y_d,z_d) is a point that is in the same cross-section as the point (x,y,z) on the dislocations with distance r_d to the latter, $G(x,y,z;x_1,y_1,z_1)$ is the Green's function corresponding to the diffusion equilibrium equation Eq. (1); $G(x,y,z;x_1,y_1,z_1) = -\frac{1}{4\pi D_v\sqrt{(x-x_1)^2+(y-y_1)^2+(z-z_1)^2}}$ when the domain is the whole three-dimensional space, the variables (x_1,y_1,z_1) describe all positions along all of the dislocation lines, and dl is the line integral element. The climb force and velocity are defined in the direction of $\boldsymbol{\xi}\times\mathbf{b}$ (i.e., the climb direction): $f_{cl}=\mathbf{f}_{PK}\cdot(\boldsymbol{\xi}\times\mathbf{b}/b)$ and $v_{cl}=\mathbf{v}\cdot(\boldsymbol{\xi}\times\mathbf{b}/b)$, where $\mathbf{f}_{PK}=(\boldsymbol{\sigma}\cdot\mathbf{b})\times\boldsymbol{\xi}$ is the Peach–Koehler force vector and $\mathbf{v}$ is the velocity vector of the dislocation.

We consider the case that the perturbations of the constituent dislocations of the tilt boundary are periodic in the y and z directions. We denote Γ' to be the collection of all the dislocation lines lying in a periodic cell, $\Lambda=(-\infty,\infty)\times(-\frac{L_y}{2},\frac{L_y}{2})\times(-\frac{L_z}{2},\frac{L_z}{2})$. The $y,z-$periodic Green's function G suitable for this problem is [27,28]

$$\begin{aligned} G(x,y,z;x_1,y_1,z_1) = {} & \frac{1}{4\pi D_v L_z}\ln\left[1-2\cos\frac{2\pi|y-y_1|}{L_y}e^{-\frac{2\pi|x-x_1|}{L_y}}+e^{-\frac{4\pi|x-x_1|}{L_y}}\right]+\frac{|x-x_1|}{2D_v L_y L_z} \\ & -\frac{1}{\pi D_v L_z}\sum_{k=1}^{\infty}\sum_{m=-\infty}^{\infty}K_0\left[\frac{2k\pi}{L_z}\sqrt{(x-x_1)^2+(mL_y+y-y_1)^2}\right]\cos\frac{2k\pi(z-z_1)}{L_z} \end{aligned} \tag{5}$$

where $K_\alpha(\cdot)$ is the modified Bessel function of the second kind. When the perturbation is uniform for all the constituent dislocations (i.e., uniform in the y direction), the period in the y direction is $L_y=D$

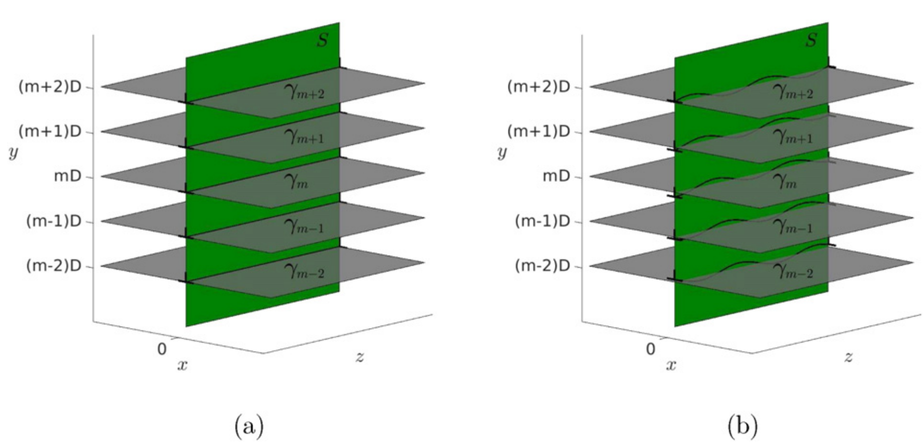

Fig. 1. (a) A low-angle symmetric tilt boundary S consisting of a regular array of edge dislocations $\gamma_j\,(j=\cdots,-2,-1,0,1,2,\cdots)$ spaced a distance D apart. (b) The constituent dislocations are perturbed in the grain boundary plane S.