

The effect of stress on grain boundary interdiffusion in a semi-infinite bicrystal

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Abstract

Chemical interdiffusion along a grain boundary in a semi-infinite bicrystal subjected to external stress normal to the boundary plane is considered. Plating out of diffusing atoms in the grain boundary partially relaxes the applied stress and modifies the driving force for diffusion. The resulting diffusion wedge formed at the grain boundary exhibits a time-independent shape, with all its linear dimensions growing with annealing time t , according to the $t^{1/3}$ law. The diffusion zone formed in the vicinity of the grain boundary is a combined result of the grain boundary diffusion and lattice drift, and is characterized by concentration discontinuities at its borders. The proposed model is applied to the analysis of liquid metal embrittlement in the Fe–In and Cu–Bi systems.

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1. Introduction

In many cases of practical interest self-diffusion and impurity diffusion along the grain boundaries (GB) occur in conditions in which high mechanical stress is applied to a bi- or polycrystalline sample. This includes creep deformation controlled by GB diffusion (Coble creep) [1], diffusional stress relaxation in thin films [2], liquid metal embrittlement (LME) [3], and dynamic embrittlement [4]. According to Herring [5], the chemical potential of atoms in the GB, which is a perfect sink/source of vacancies, is modified by

$$\Delta\mu = -\sigma\Omega \quad (1)$$

where $\Delta\mu$ is the change in chemical potential due to the normal tensile traction σ at the GB, and Ω is the atomic volume. In this equation all higher-order contributions of the stress tensor components to $\Delta\mu$ have been neglected.

In this approximation, for any arbitrary stress field only the traction normal to the GB plane modifies the chemical potential of GB atoms. Eq. (1), implying that the gradients of normal stress modify the driving force for GB diffusion, is the basis for the quantitative analysis of the diffusion in stressed GB. However, it is often overlooked that the normal stress at the GB can be relaxed by the wedging effect of diffusing atoms which are plated out in the GB [6]. For samples of finite size, the wedging effect may lead to the steady-state deformation regime in which the lattice drift normal to the GB does not depend on location. Such a steady-state regime was considered in the analyses of GB grooving in thin foils [7] and creep deformation of bamboo nanowires [8]. A more general analysis which is not limited by a steady-state regime requires simultaneous treatment of diffusion and elasticity problems that take into account the wedging effect. This was done recently by Gao and co-workers, who considered self-diffusion controlled formation of “diffusion wedges” that relax tensile internal stresses in thin films deposited on rigid substrates [9,10]. The aim of the present work is to extend the analyses of Gao et al. to the two-component system. Having the appli-

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cations to LME and dynamic embrittlement in mind, the study considers a semi-infinite bicrystal with the unlimited source of diffusant atoms at the surface.

2. The model

A semi-infinite bicrystal of solid phase B subjected to a tensile stress σ_0 normal to the GB is considered (see Fig. 1). Component A penetrates the GB in phase B in a way that does not limit either the supply of A atoms to the GB or the removal of B atoms from the GB at the A/B interface. (It is assumed that A and B form a substitutional solid solution in the GB.) This may correspond to a macroscopic droplet of liquid phase A deposited on the surface of B (LME), or to the supply of A from the A -rich vapor phase and removal of B atoms from the GB by a fast mechanism of surface diffusion. Furthermore, the diffusion in the bulk is neglected. This corresponds to temperatures below $\sim 0.4T_m$ (where T_m is the melting temperature of B). The divergence of the diffusion fluxes along the GB leads to the plating out of additional material there in the form of an extra material wedge. This wedge partly relaxes the normal stress at the GB, which gives rise to normal stress variations along the GB, contributing to the driving force for GB diffusion of both components.

In continuous limit, a layer of new material of the thickness $w(y, t)$ (here y is the coordinate along the GB, and t is the annealing time) plated out in the GB can be represented as an ensemble of edge dislocations with the Burgers vector density $\partial w/\partial y$ [9]. In this approximation, further inward diffusion of A and thickening of the diffusion wedge at the GB correspond to the inward climb of these dislocations. The corresponding normal stress at the GB can be written as [9]:

$$\sigma(y, t) = \sigma_0 - E^* \int_0^\infty K(y, z) \frac{\partial w(z, t)}{\partial z} dz \quad (2)$$

where $E^* = \frac{E}{4\pi(1-\nu^2)}$ is the equivalent elastic module, and

$$K(y, z) = \frac{1}{y-z} + \frac{1}{y+z} - \frac{6y}{(y+z)^2} + \frac{4y^2}{(y+z)^3} \quad (3)$$

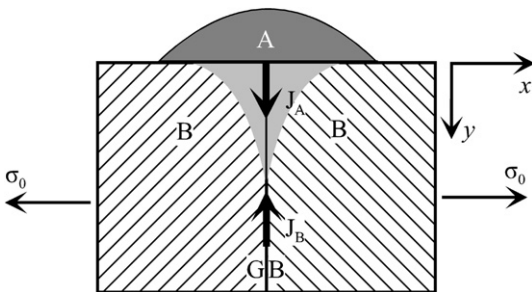


Fig. 1. A bicrystal of B with external stress σ_0 applied normal to the GB. The A atoms diffuse from the liquid droplet along the GB.

The atomic fluxes of the components along the GB can be represented as the sum of two contributions associated with the concentration and normal stress gradients:

$$J_A = -\delta D_{\text{gb}} \frac{\partial c_{\text{gb}}^A}{\partial y} + \frac{\delta D_{\text{gb}} \Omega}{kT} c_{\text{gb}}^A \frac{\partial \sigma}{\partial y} \quad (4a)$$

$$J_B = -\delta D_{\text{gb}} \frac{\partial c_{\text{gb}}^B}{\partial y} + \frac{\delta D_{\text{gb}} \Omega}{kT} c_{\text{gb}}^B \frac{\partial \sigma}{\partial y} \quad (4b)$$

where δD_{gb} is the product of the GB thickness and the diffusion coefficient along the GB (supposed to be identical for both components), Ω is the atomic volume (also supposed to be the same for both components), $c_{\text{gb}}^{A,B}$ are the GB concentrations (at. m⁻³) of components A and B :

$$c_{\text{gb}}^A + c_{\text{gb}}^B = 1/\Omega \quad (5)$$

Note that, contrary to the previous analyses of the problem [6], the normal stress at the GB affects the diffusion fluxes of both components. Also, in this model, the pressure dependence of the GB diffusivities is neglected. The conditions of mass conservation for both components can be written in the following form:

$$\delta \frac{\partial c_{\text{gb}}^i}{\partial t} = -\frac{\partial J_i}{\partial y} - c_x^i \frac{\partial w}{\partial t}, \quad i = A, B \quad (6a)$$

$$c_x^i = \begin{cases} c_{\text{gb}}^i & \dot{w} > 0 \\ c_{\text{bulk}}^i & \dot{w} < 0 \end{cases} \quad (6b)$$

where c_{bulk}^i are the bulk concentrations of the components (for this case $c_{\text{bulk}}^A = 0$, $c_{\text{bulk}}^B = 1/\Omega$). The second term on the right-hand side (RHS) of Eq. (6a) describes the plating out (or in) of the material at the GB to (or from) the surrounding lattice.

Combining Eqs. (4)–(6) yields

$$\frac{\partial w(y, t)}{\partial t} = -\frac{\delta D_{\text{gb}} \Omega}{kT} \frac{\partial^2 \sigma(y, t)}{\partial y^2} \quad (7)$$

It is the assumption of equal GB diffusivities and atomic volumes of the two components that allows the equation for $w(y, t)$ to be decoupled from the GB concentrations. In the general case, the equation for $w(y, t)$ will include the functions c_{gb}^i , their derivatives and the atomic volumes of the components. Solving it is beyond the scope of the present work. Eq. (7), together with Eq. (2), describes the stress distribution in the system and the kinetics of the diffusion wedge growth. After solving these equations, one can return to Eqs. (4) and (6) to find the distribution of the components in the diffusion zone.

3. Stress distribution and diffusion wedge shape

Taking a time derivative of Eq. (2) and substituting the resulting relationship into Eq. (7) yields an integro-differential equation for stress:

$$\frac{\partial \sigma(y, t)}{\partial t} = G \int_0^\infty K(y, z) \frac{\partial^3 \sigma(z, t)}{\partial z^3} dz \quad (8)$$

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