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Modeling Grain Boundary Mobility during Dynamic Recrystallization of Metallic Alloys

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Abstract. A simple analytical model is proposed for estimating grain boundary mobility during dynamic recrystallization in metallic alloys. The combined effects of solutes (solute drag) and second phase particles (Zener pinning) on mobility are considered. The approach is based on (and is consistent with) a recently published mesoscale model of discontinuous dynamic recrystallization. The dependence of grain boundary mobility on solute concentration and particle size is summarized in the form of two-dimensional maps.

Introduction

Grain boundary migration plays an important role in dynamic recrystallization because it is one of the main parameters controlling the final grain size after hot working of a material. In metallic alloys, the grain boundary mobility M is generally decreased by both solute atoms (solute drag effect) and second phase particles (Zener pinning) [1]. Within the range of large grain-boundary velocities involved in classical "discontinuous" dynamic recrystallization (DDRX), M is expected to drop monotonically with increasing solute concentration. By contrast, the *local* grain boundary migration rate either falls to zero or remains unchanged according to whether the driving force is less or greater than the Zener pressure P_z . Such discontinuous behaviour precludes any straightforward introduction of Zener pinning into models of DDRX, and it is therefore necessary to estimate an *average* value of the mobility pertaining to a whole grain over its lifetime.

Mesoscale Power-Law DDRX Model

In a mesoscale "average field" model for DDRX recently published [2, 3], each grain is considered as a spherical "inclusion" of current diameter D and (homogeneous) dislocation density ρ interacting with a matrix of average dislocation density $\bar{\rho}$. The grain size changes according to:

$$dD/d\varepsilon = (2M\tau/\dot{\varepsilon})(\bar{\rho} - \rho), \quad (1)$$

in which ε and $\dot{\varepsilon}$ are the strain and strain rate, respectively, and $\tau \approx \mu b^2$ is the line energy of dislocations. According to Eq. 1, each grain grows whenever its dislocation density is less than $\bar{\rho}$, and shrinks in the opposite case. The evolution of dislocation density reflects strain hardening and dynamic recovery. Various equations have been proposed to describe such phenomena; most of them involve numerical computations. In the present work, however, the following simple power law is used, because it leads to closed-form analytical expressions:

$$d\rho/d\varepsilon = H^{v+1}/\rho^v, \quad (2)$$

in which $v \geq 0$, and H has the dimension of dislocation density (μm^{-2}). Note that Eq. 2 is associated with the classical macroscopic (power law) *Swift* equation $\sigma = K(\varepsilon + \varepsilon_1)^{n_s}$, in which K , ε_1 , and the macroscopic strain-hardening parameter $n_s = 1/(2 + 2v)$ are constants. During the *steady state* of DDRX, $\bar{\rho}$ remains constant. Integration and combination of Eqs. 1 and 2 then lead to:

$$D = \frac{2M\tau}{\dot{\varepsilon}} \left(\frac{\rho}{H} \right)^{v+1} \left(\frac{\bar{\rho}}{v+1} - \frac{\rho}{v+2} \right). \quad (3)$$

When the grain vanishes, its dislocation density reaches its maximum value

$$\rho_{\text{end}} = \frac{v+2}{v+1} \bar{\rho} \quad (4)$$

obtained by setting $D = 0$ in Eq. 3. (The other solution, $\rho = 0$, corresponds to the nucleation of a new grain.)

Grain Boundary Mobility during DDRX of an Alloy Containing Precipitates

When stable, incoherent *precipitates* are present in the material, they exert a drag (Zener) pressure P_z that opposes grain boundary motion. Setting $\rho_z = P_z/\tau$,

- if $|\bar{\rho} - \rho| \leq \rho_z$, the migration rate is zero because the boundary is pinned by precipitates, and therefore $M = 0$;
- if $|\bar{\rho} - \rho| > \rho_z$, the boundary moves with mobility M_1 (the mobility in the absence of Zener drag), possibly affected by solute atoms (see below), as illustrated in Figure 1. (However, M_1 is likely to depend also on the Zener pressure, a question which is left for later investigation.)

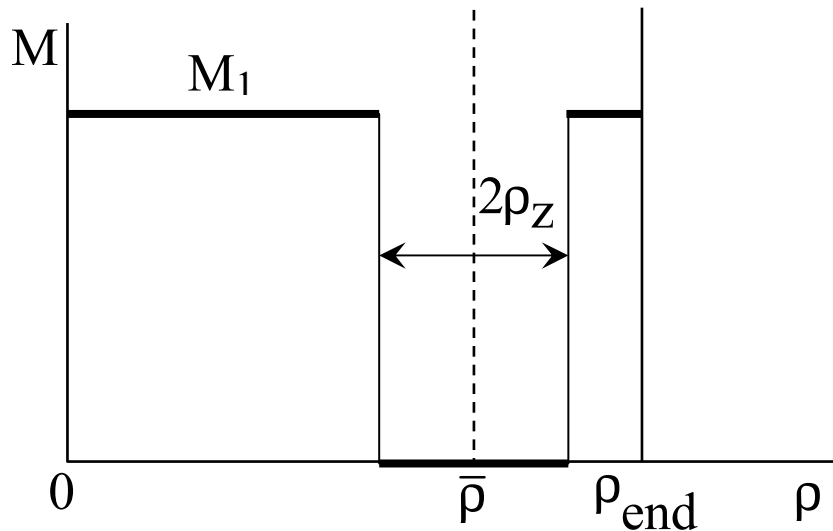


Figure 1. Schematic dependence of mobility with respect to the dislocation density in the grain

The average mobility pertaining to the grain over its lifetime (or, equivalently, pertaining to the whole set of grains under the DDRX steady state) is then given by:

$$M = S_1/S, \quad \text{in which } S_1 = \int_0^{\rho_{\text{end}}} M(\rho) D(\rho)^2 \rho^v d\rho \quad \text{and} \quad S = \int_0^{\rho_{\text{end}}} D(\rho)^2 \rho^v d\rho \quad (5)$$

In Eq. 5, the average of $M(\rho)$ is weighted by the current surface of the grain. The additional factor ρ^v occurs because of the change of variable from time t to dislocation density ρ . Two cases are distinguished for evaluating the integral for S_1 :

- If $\bar{\rho} + \rho_z \leq \rho_{\text{end}}$, *i.e.*, $\rho_z \leq \bar{\rho}/(v+1)$,

$$S_1 = M_1 \int_0^{\bar{\rho}-\rho_z} D(\rho)^2 \rho^v d\rho + M_1 \int_{\bar{\rho}+\rho_z}^{\rho_{\text{end}}} D(\rho)^2 \rho^v d\rho \quad (6a)$$

- If $\bar{\rho} + \rho_z > \rho_{\text{end}}$, *i.e.*, $\rho_z > \bar{\rho}/(v+1)$,

$$S_1 = M_1 \int_0^{\bar{\rho}-\rho_z} D(\rho)^2 \rho^v d\rho \quad (6b)$$

Closed formed expressions are then obtained for the above integrals using Eq. 3 (steady state DDRX). Figure 2 shows that M drops rapidly with increasing Zener pressure P_z for given deformation conditions, *i.e.*, a given $\bar{\rho}$. However, the influence of precipitates decreases for low values of v , *i.e.*, when strain hardening is strong (per Eq. 2).

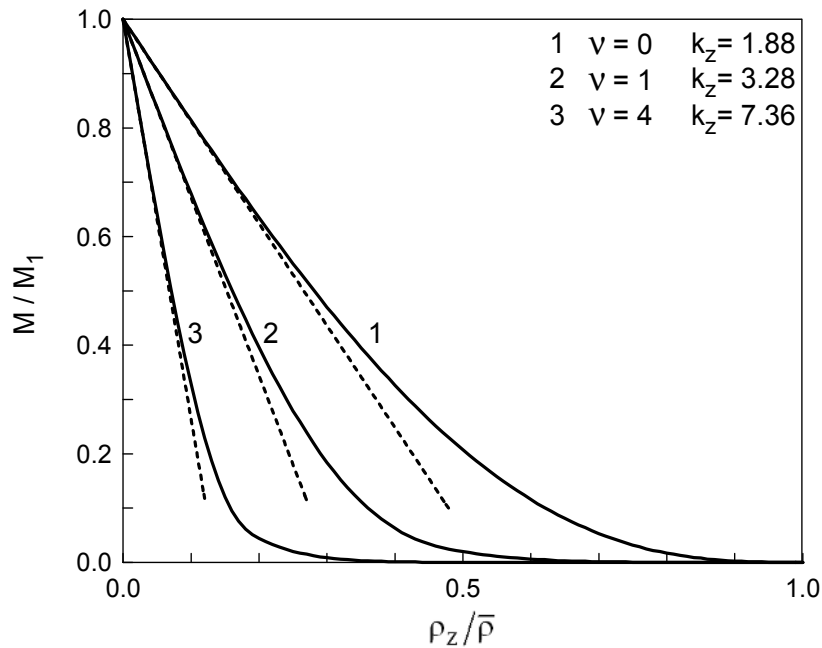


Figure 2. Dependence of the grain boundary mobility M on Zener pressure ρ_z (solid lines) and the corresponding linear approximations at low values of ρ_z (broken lines). Numerical values of the slope, k_z (Eq. 7), are given for $v = 0, 1$, and 4 , *i.e.*, for $n_s = 0.5, 0.25$, and 0.1 , respectively

It appears that the linear approximations of M given by the initial slopes of the curves in Figure 2 are quite acceptable for $M/M_1 > 0.3$. This is relevant because DDRX requires sufficient grain boundary mobility for it to occur. For $\rho_z/\bar{\rho} \ll 1$, first order polynomial expansion of the integrals in Eq. 6a leads to a relation for M/M_1 :

$$M/M_1 = 1 - k_z (\rho_z/\bar{\rho}) \quad \text{in which} \quad k_z = (3v+3)(3v+4)(3v+5)(v+1)^{3v+3}/(v+2)^{3v+5} \quad (7)$$

It is interesting to note that a linear equation similar to the above has been recently proposed by Hutchinson *et al.* [1].

Overall Expression for the Grain Boundary Mobility

The influence of *solute*s on the grain boundary mobility can be described by the classical equation:

$$M_1 = \frac{M_0}{1 + \beta C_m} \quad (8)$$

pertaining to the range of large migration rates occurring during DDRX [4]. Here, M_0 is the mobility in the pure metal, C_m is the atomic concentration (atoms/m³) of solute in the matrix, and β a constant. It is more convenient to write Eq. 8 in a slightly modified form:

$$M_1 = \frac{M_0}{1 + \alpha (C_m/C_s)} \quad (8a)$$

in which the maximum (*saturation*) solute concentration C_s (which is a function of temperature, and may be modified under deformation conditions) has been introduced, and α is a non-dimensional constant. Contrary to the case of Zener pinning, it is not possible here to use a linear expansion of Eq. 8a, since C_m/C_s is expected to vary over the whole range between 0 and 1, or even exceed unity (supersaturation).

The grain boundary mobility in particle and solute-containing metals undergoing DDRX is therefore obtained by combining Eqs. 7 (assuming here that its validity range extends up to $M = 0$) and 8a, viz.,

$$M = M_0 \frac{1 - k_z (\rho_z/\bar{\rho})}{1 + \alpha (C_m/C_s)} \quad (9)$$

Particle Size and Solute Concentration Dependence of Grain Boundary Mobility

Assuming spherical particles, the Zener pressure is given by [4]:

$$P_z = (\pi/2) \gamma n d^2 \quad (10)$$

in which γ is the surface energy of the precipitates, n is the number of precipitates per unit volume, and d denotes their diameter. In addition, alloy atom conservation leads to the following equation:

$$C_m + (\pi/6) d^3 n C_p = C \quad (11)$$

in which C_p is the concentration (atoms/m³) of alloy element in each precipitate, and C is the overall alloy concentration. Combining Eqs. 10 and 11 yields:

$$P_z = 3\gamma \frac{C - C_m}{C_p d}. \quad (12)$$

Eq. 9 can then be written in the form:

$$M = M_0 \frac{1 - \delta k_z \frac{C/C_s - C_m/C_s}{d}}{1 + \alpha C_m/C_s} \quad \text{with} \quad \delta = \frac{3\gamma}{\tau \bar{\rho} C_p/C_s} \quad (13)$$

Here, δ is a constant (with units of length) for given deformation conditions. The dependence of M/M_0 on d and C_m can then be plotted in a two-dimensional diagram, for given overall concentration C . However, an additional condition must be fulfilled, *viz.*, $L/d > (L/d)_c > 1$, in which L denotes the average center-to-center distance between precipitates, and the critical ratio $(L/d)_c$ means that the Zener pinning theory is likely to hold only for sufficiently widely-spaced precipitates. Using $n = 1/L^3$, Eq. 11 can then be recast in the form:

$$\frac{L}{d} = \left(\frac{\pi}{6} \frac{C_p/C_s}{C/C_s - C_m/C_s} \right)^{1/3}. \quad (14)$$

Substitution of this expression for L/d in the above inequality and solving for C_m/C_s leads to the condition:

$$\frac{C_m}{C_s} > \frac{C}{C_s} - \frac{\pi}{6} \frac{C_p/C_s}{(L/d)_c^3} \quad (15)$$

to be fulfilled by the solute concentration C_m .

An example calculation of the grain-boundary mobility as a function of material and alloy parameters is shown in Figure 3. For this example, $C_p = 2.23 \times 10^{28}$ atoms/m³ was estimated for the case of niobium in hexagonal Ni₃Nb precipitates, and it was assumed that $C/C_s = 0.5$ (“undersaturated” alloy concentration) and $(L/d)_c = 1.5$. Other input parameters are specified in the caption. In the cross-hatched area, the grain boundary mobility is zero. M values are meaningful only for $L/d > (L/d)_c = 1.5$, according to the above analysis. Furthermore, the diagram exhibits a critical particle diameter d_c . For $d < d_c$, the mobility *increases* with C_m (because the particle spacing becomes larger, thus weakening the Zener pressure). For $d > d_c$, the mobility *decreases* with increasing C_m because solute effects predominate. For $d = d_c$, grain boundary mobility is *independent* of the solute concentration.

Concluding Remarks

A model has been developed to estimate the combined effect of solutes and precipitates on the grain boundary mobility under conditions of dynamic recrystallization. Although the various material parameters are not well known, it nevertheless indicates general trends and orders of magnitude that can be used as inputs for modeling DDRX in metallic alloys. Conversely, a recently-published, mesoscale model of DDRX enables the mobility to be determined from the steady-state flow stress and average grain size measurements [3]. It is thus also possible to estimate unknown material parameters from such data.

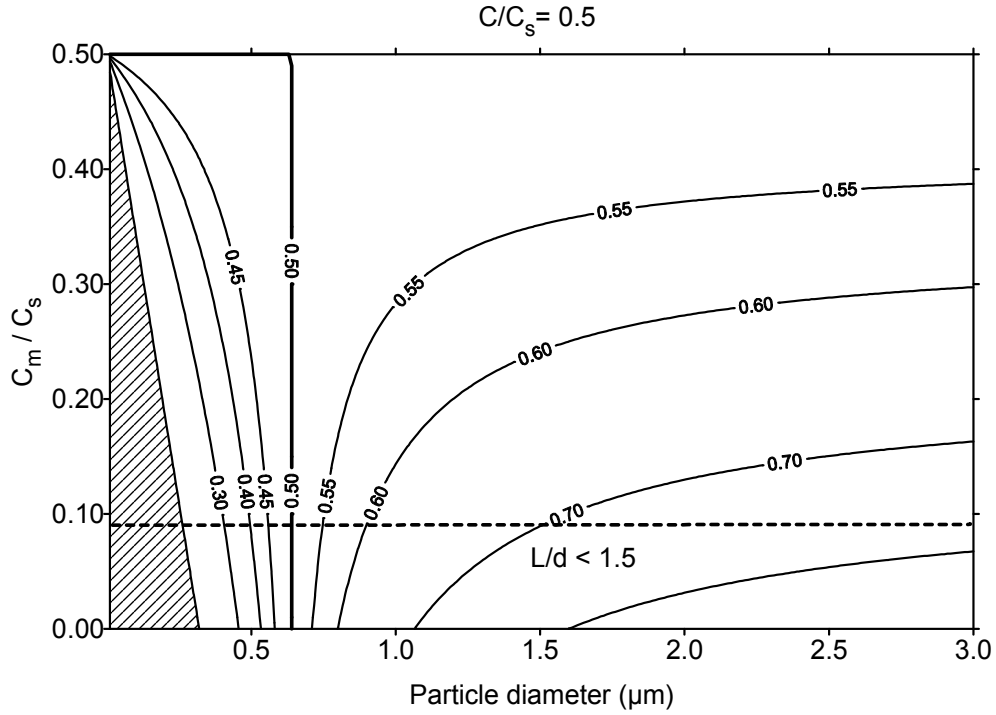


Figure 3. Diagram showing the dependence of the grain boundary mobility (M/M_0) on the particle diameter and solute concentration for an overall alloy concentration $C/C_s = 0.5$. Other parameters assumed for the model calculations comprised $\gamma = 0.5 \text{ J/m}^2$; $k_z = 1.88$ (associated with $v = 0$ and a macroscopic strain hardening exponent of 0.5); $\tau = 3.306 \times 10^{-9} \text{ J/m}$ and $\bar{p} = 510.2 / \mu\text{m}^2$ (both estimated for a Ni-Nb alloy at 900°C , 10^{-1} s^{-1}); $C_p = 2.23 \times 10^{28} \text{ atoms/m}^3$ (for niobium in hexagonal Ni_3Nb); $C_s = 0.85 \times 10^{28} \text{ atoms/m}^3$ (for niobium in nickel at 900°C); and $\alpha = 2$

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