Modelling grain boundary migration during geometric dynamic recrystallization

M. A. Martorano *; A. F. Padilha *

* Department of Metallurgical and Materials Engineering, University of São Paulo, São Paulo, Brazil

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Modelling grain boundary migration during geometric dynamic recrystallization

M.A. Martorano* and A.F. Padilha

Department of Metallurgical and Materials Engineering, University of São Paulo, São Paulo, Brazil

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High-angle grain boundary migration is predicted during geometric dynamic recrystallization (GDRX) by two types of mathematical models. Both models consider the driving pressure due to curvature and a sinusoidal driving pressure owing to subgrain walls connected to the grain boundary. One model is based on the finite difference solution of a kinetic equation, and the other, on a numerical technique in which the boundary is subdivided into linear segments. The models show that an initially flat boundary becomes serrated, with the peak and valley migrating into both adjacent grains, as observed during GDRX. When the sinusoidal driving pressure amplitude is smaller than \( \frac{2}{C^{25}} \), the boundary stops migrating, reaching an equilibrium shape. Otherwise, when the amplitude is larger than \( 2\pi \), equilibrium is never reached and the boundary migrates indefinitely, which would cause the protrusions of two serrated parallel boundaries to impinge on each other, creating smaller equiaxed grains.

**Keywords:** geometric dynamic recrystallization; grain boundary migration; serration; modelling; grain boundaries; numerical modelling; recrystallization

1. Introduction

Geometric dynamic recrystallization (GDRX) has been described as the formation of equiaxed grains by the migration and impingement of serrated high-angle grain boundaries belonging to grains elongated by hot deformation [1]. During GDRX, the peaks of grain boundary serrations on opposite sides of one grain come into contact with each other, causing the grain to pinch off and be divided into a few smaller, equiaxed grains similar to those observed after discontinuous dynamic recrystallization [2–5]. One essential condition for the occurrence of GDRX is the formation of serrations, also termed undulations or protrusions, at the high-angle grain boundaries. There is experimental evidence showing that serrations form by local migration of high-angle grain boundaries at the junctions with the subgrain boundaries created by dynamic recovery [4]. McQueen et al. [4] also suggested that, as opposed to discontinuous recrystallization, the protrusions at a serrated high-angle grain boundary moved into both adjacent grains down their subgrain boundary structures. As a result, the wavelength of serrations is highly correlated with the subgrain size.

*Corresponding author. Email: martoran@usp.br
The GDRX has been observed in several types of materials: high purity Al [6] and Cu [7]; pure Zr [8,9]; Al–5.2Mg [10]; Al–5Mg and 6015 Al alloys [2]; Mg–2.8Al–0.9Zn and Mg–5.7Zn–0.65Zr alloys [11,12]. Although the mechanisms leading to GDRX is relatively well understood and have been observed in different metals and alloys, no attempt to model the grain boundary migration during GDRX exists in the literature. Recently, Martorano et al. [13] proposed a kinetic equation to predict the movement of grain boundaries in two dimensions, showing the growth of grain boundary protrusions that lead to serrated grain boundaries. In their model, the grain boundary was subjected to a driving pressure due to boundary curvature and to a driving pressure that varied sinusoidally along the boundary. Using this model, the formation of serrations at high-angle grain boundaries during recrystallization was shown [13]. The boundary shape was seen to reach a steady state in relation to a moving reference frame.

The model results shown by Martorano et al. [13] do not strictly apply to the migration of a serrated boundary during GDRX, because all parts of this boundary moved into only one adjacent grain, as a mechanism of discontinuous recrystallization. The adopted sinusoidal driving pressure with non-zero mean value caused the grain boundary to move completely into only one adjacent grain.

In the present work, the kinetic equation derived by Martorano et al. [13], and the least square-normal and curvature (LSNC) model proposed by the same authors [14] are used to model the local migration of high-angle grain boundaries during GDRX. The mean value of the sinusoidal driving pressure, however, was now assumed zero, enabling more realistic predictions of the evolution of the grain boundary shape.

2. Mathematical modelling

The two-dimensional physical model adopted in the present work to predict the migration of a high-angle grain boundary during GDRX is explained in Figure 1. In Figure 1a, an optical micrograph by Kassner [15] is given, showing the microstructure for high-purity aluminium (99.999% purity) deformed at elevated temperature and quenched during GDRX. There are elongated grains containing one or two subgrains along the grain width. Humphreys and Hatherly [1] have suggested that one condition for GDRX is that the subgrain size should be approximately equal to the grain thickness.

In Figure 1a, some regions that closely represent the physical model proposed in Figure 1c are indicated by rectangles to show the relation between the high-angle grain boundary shape and the subgrains on each side of the boundaries. Region A is illustrated in detail in Figure 1b, where subgrain walls are also indicated on each side of the boundary. Finally, the physical model proposed in the present work to represent the grain boundary migration depicted in Figure 1b during GDRX is given in Figure 1c.

In this model, the boundary is initially flat and subjected to a driving pressure $F$ caused by dislocation walls (subgrain boundaries) located on both sides of the boundary, inside the adjacent grains. The driving pressure $F$ varies sinusoidally along the boundary as follows

$$F = \Delta F \sin \frac{2\pi x}{\lambda}$$

(1)
where $x$ is the coordinate along the boundary; $\Delta F$ is the amplitude; and the wavelength $\lambda$ equals the separation distance between dislocation walls. The boundary shape is defined by $y = y(x, t)$, where $t$ is time. Note that this driving pressure differs from that assumed by Martorano et al. [13], because it is symmetric in relation to the grain boundary position.

Two types of mathematical models were used to predict the grain boundary migration in the physical model of Figure 1c. The first is based on the kinetic equation derived by Martorano et al. [13], which was developed from the following classical kinetic equation of grain boundary migration [16,17]:

$$v_n = M\left(\frac{\sigma}{R} + F\right)$$

(2)
where \( v_n \) is the local normal velocity of the boundary; \( R \) is the local radius of curvature of the boundary; \( \sigma \) is the boundary energy per unit area; and \( M \) is the boundary mobility. This equation was applied to model the migration of a two-dimensional boundary described by \( y = y(x, t) \). The normal velocity was expressed as \( v_n = \left( \frac{\partial y}{\partial t} \right) \left( 1 + y^2 \right)^{-1/2} \), where \( \frac{\partial y}{\partial t} \) is the boundary velocity in the \( y \) direction and \( (1 + y^2)^{-1/2} \) is the magnitude of the component of the boundary normal in the \( y \) direction. The radius of curvature, \( R \), can be calculated by the well-known relation \( R = \left( 1 + y^2 \right)^{3/2} / y \) [18]. Substituting the expressions for \( v_n \), \( R \) and the driving pressure from Equation (1) into Equation (2) yields the following kinetic equation in dimensionless form [13]

\[
\frac{\partial y^*}{\partial t^*} = \dot{y}^* \left( 1 + \dot{y}^{*2} \right)^{-1} + \Delta F^* \sin(2\pi \lambda^* \left( 1 + \dot{y}^{*2} \right)^{1/2})
\]

where \( \dot{y}^* = \frac{\partial y^*}{\partial x^*} \), and the dimensionless quantities were defined as: \( x^* = x / \lambda \); \( y^* = y / \lambda \); \( t^* = M\sigma / \lambda^2 \); \( \Delta F^* = \lambda \Delta F / \sigma \). Each term in Equation (3) has an equivalent meaning to the terms in Equation (2): the first term on the right-hand side represents the pressure owing to the boundary curvature, whereas the second term is a result of the sinusoidal driving pressure \( F \). Equation (3) was used to calculate the time evolution of the boundary, \( y^*(x^*, t^*) \), in one period of the driving pressure, i.e., periodic boundary conditions were used. The initial condition was given by \( y^*(x^*, 0) = 0 \). As explained in [13], Equation (3) was solved numerically by the implicit formulation of the finite difference method using a mesh of 801 equally spaced nodes [19]. The numerical solution of Equation (3) becomes increasingly more difficult as parts of the boundary become approximately perpendicular to the \( x \) axis, because a large density of mesh nodes is required to represent these boundary segments.

A second type of mathematical model was also used to predict the grain boundary migration in the conditions where the kinetic equation (Equation (3)) was difficult to be solved numerically. This model, referred to as the least square-normal and curvature (LSNC) model, was proposed by Martorano et al. [14] to predict the migration of boundaries in problems where the pressure due to curvature and boundary energy is important. This model, based on a method to track free-surfaces during fluid flow, uses a mesh of two-dimensional rectangular or square cells. Each portion of the boundary within one cell is represented by a line segment. To calculate the local curvature at the portion of the boundary within a cell, a quadratic equation is fit to the mid-points of the boundary segments located within the cell and its nearest neighbours. Then the classical kinetic equation (Equation (2)) is applied at each boundary segment to calculate its velocity in the normal direction, enabling the determination of the boundary segment displacement. As in the finite difference solution of the kinetic equation, the boundary was assumed initially flat and periodic boundary conditions were also adopted at the left and right-hand side walls of the two-dimensional calculation domain.

The LSNC model is robust and can be used to track the migration of any type of grain boundary, including those with some parts perpendicular to the \( x \) axis, which pose severe difficulties to the numerical solution of Equation (3). A two-dimensional mesh, however, is necessary for the LSNC model, requiring more computer time than that for the finite difference solution of Equation (3), in which a one-dimensional mesh can be used. In the calculations of the present work, square cells of dimensionless size 1/150 were used...
in the mesh. The exact number of cells varied with the size of the domain in the \( y^* \) direction, but the cell size was the same in all simulations. The dimensionless time step of the numerical method was \( 2 \times 10^{-5} \). Further details about the LSNC model can be found in [14].

3. Boundary migration during geometric dynamic recrystallization

The time evolution of the initially flat grain boundary calculated with the kinetic equation and the LSNC model for \( \Delta F^* = 5 \) and \( \Delta F^* = 7 \) is shown in Figure 2a and b, respectively. The results obtained with these models, based on completely different modelling techniques, agree very well, confirming the convergence to the solution of the mathematical problem. For both \( \Delta F^* \) values, the boundary protrusions migrate into the two adjacent grains (positive and negative \( y^* \) coordinates), as observed during GDRX. Owing to the driving pressure \( F^* \), which has absolute maximum values at \( x^* = 1/4 \) and \( 3/4 \), but is zero at \( x^* = 0, 1/2 \) and 1, the boundary remains fixed at \( x^* = 0, 1/2 \) and 1, but its peak and valley are located at \( x^* = 1/4 \) and \( 3/4 \), respectively, attaining the serrated shape observed at the high-angle grain boundaries during GDRX.

For \( \Delta F^* = 5 \) (Figure 2a), the initially flat boundary migrates, reaches a serrated shape, and stops, no longer changing its shape (i.e., reaching an equilibrium shape), until \( \tau^* = 0.3 \). On the other hand, for \( \Delta F^* = 7 \) (Figure 2b), after becoming serrated, the boundary migrates continuously, never reaching an equilibrium shape. The protrusions become increasingly elongated, but the shape at the peak and valley no longer changes. This type of behaviour might be the one observed during GDRX and might cause the serrations of two approximately parallel grain boundaries to contact and pinch off, forming equiaxed grains, as described previously.

When \( \Delta F^* = 7 \), the calculated boundary is shown for both models only until \( \tau^* = 0.2 \). After this time, the numerical solution of the kinetic equation is difficult, because the boundary is almost perpendicular to the \( x^* \) axis at \( x^* = 0, 1/2 \) and 1, requiring a much larger density of node points for the finite difference method. Therefore, only the LSNC model results are shown for \( \tau^* > 0.2 \).

The existence or not of an equilibrium shape during grain boundary migration is examined using Equation (3) by forcing \( \partial y^*/\partial \tau^* = 0 \), which gives

\[
\dot{y}^* + \Delta F^* \sin(2\pi x^*)(1 + \dot{y}^*)^{3/2} = 0
\]

In this equation, the driving pressure \( F^* \) is equilibrated with the pressure caused by the boundary curvature and the boundary no longer migrates.

With the periodic boundary conditions adopted for the two models in the present work, the calculated boundaries naturally remained fixed at \( x^* = 0 \) and 1 (Figure 2). Therefore, an analytical solution to Equation (4) was obtained using, as boundary conditions, \( y^*(x^* = 0, \tau^*) = y^*(x^* = 1, \tau^*) = 0 \). The solution is

\[
y^*_s = \frac{1}{4\pi} \ln \left\{ \frac{0.5[1 - (2\pi/\Delta F^*)^2]}{\cos^2(2\pi x^*) + \sin^2(2\pi x^*)[\cos^2(2\pi x^*) - \cos^2(2\pi x^*)]^{1/2} + 0.5[1 - (2\pi/\Delta F^*)^2]} \right\}
\]

(5)
where $y^*_s$ is the coordinate of the boundary at its equilibrium shape. As can be concluded from Equation (5), the equilibrium profile can only be completely calculated when $\Delta F^* < 2\pi$. Actually, when $\Delta F^* > 2\pi$ the peaks and valleys of the serrated boundary migrate indefinitely, never reaching an equilibrium shape, as shown in Figure 2b for $\Delta F^* = 7$. In Figure 2a, on the other hand, $\Delta F^* = 5$ ($< 2\pi$) and an equilibrium shape is reached. Several equilibrium boundary shapes, calculated with Equation (5) for $\Delta F^* < 2\pi$, are shown in Figure 3. An increase in $\Delta F^*$ increases the amplitude of the boundary serration at equilibrium, as expected. The equilibrium shapes obtained with the LSNC model show excellent agreement with those calculated with Equation (5).

The total amplitude of the boundary serration, defined as $\Delta y^* = y^*(x^* = 1/4) - y^*(x^* = 3/4)$, and the normal migration velocity, $V^*$, calculated as a function of time at

Figure 2. Time evolution of grain boundaries calculated with the kinetic equation and the LSNC model for $\Delta F^* = (a) 5$, and (b) 7.
the peak \(x^* = 1/4\) with the LSNC model and with the kinetic equation (Equation (3)) are given in Figure 4. The amplitude reaches a constant value and the velocity decreases down to zero for \(\Delta F^* \leq 5\) after \(t^* \approx 0.3\), when equilibrium is reached. For \(\Delta F^* = 7\) and 10, the boundary amplitude increases continuously and the migration velocity reaches a constant value, showing that the boundary will never stop, as discussed previously for \(\Delta F^* > 2\pi\).

The time evolution of the dimensionless radius of curvature, defined as \(R^* = R/\lambda\), calculated at the boundary peak \((x^* = 1/4)\) with the two models is shown in Figure 5. Since the boundary is initially flat, \(R^* \to \infty\) as \(t^* \to 0\), but \(R^*\) decreases as the boundary changes its shape from flat to sinusoidal or serrated. For \(\Delta F^* \leq 5\), the boundary stops migrating and \(R^*\) becomes constant, equal to a critical radius \(R^*_\text{crit}\), after \(t^* \approx 0.1\). When \(R = R^*_\text{crit}\), the magnitude of the sinusoidal driving pressure equals that of the curvature pressure in the opposite direction, resulting in the equilibrium of pressures. The value of \(R^*_\text{crit}\) is calculated applying the classical kinetic equation (from which Equation (3) was derived) at the peak of the serration, yielding

\[
|R^*_\text{crit}| = 1/\Delta F^*
\]  

In Figure 5, for \(\Delta F^* \leq 5\), the radius of curvature at the peak, \(R^*\), decreases to the value of \(R^*_\text{crit}\) calculated with Equation (6), indicated by the dashed line for each \(\Delta F^*\). For \(\Delta F^* = 7\) and 10, however, \(R^*\) decreases to \(1/2\pi\) and remains constant thereafter. Since \(R^* = 1/2\pi > R^*_\text{crit}\), the pressure due to curvature \((1/R^*)\) is smaller than the sinusoidal driving pressure \((\Delta F^*)\), preventing an equilibrium shape to be reached, i.e., the boundary never stops, resulting in the elongated protrusions of Figure 2b. Note that, when \(\Delta F^* > 2\pi\), the minimum radius of curvature that the boundary reaches at the peak and valley is \(1/2\pi\), regardless of the \(\Delta F^*\) value.

Although serrated boundaries have been observed during GDRX in several metals and alloys, only crude estimates of the driving pressure due to subgrains can be obtained in

Figure 3. Boundaries at the equilibrium shape calculated with the kinetic equation (Equation (5)) and the LSNC model for several driving pressure amplitudes, \(\Delta F^*\).
these cases, because the subgrain structure is not reported. In the work on hot-deformation of Al-5.8 at.% Mg alloy by Henshall et al. [10], the bulk driving pressure in dimensionless form, \( F^* = \frac{F}{\sigma} \), was estimated by Martorano et al. [13]. This dimensionless pressure, which was considered to stem mainly from the energy stored in the subgrain structure, was in the range between 7 and 9. Since \( F^* \) changes sinusoidally, \( \Delta F^* \) is probably larger than 7, i.e., \( \Delta F^* > 2\pi \). Consequently, a high-angle grain boundary would migrate unimpeded without reaching equilibrium until contacting another serrated boundary, leading to GDRX.
4. Concluding remarks

Two types of two-dimensional models based on completely different numerical techniques were used to predict the migration of high-angle grain boundaries during geometric dynamic recrystallization (GDRX). Both models showed that when a sinusoidal driving pressure with zero-mean value is assumed, the boundary becomes serrated and its peak and valley migrate into the two adjacent grains, as observed during GDRX. When the amplitude of the dimensionless driving pressure, $\frac{\Delta F^*}{C_1F/C_3}$, the boundary stops migrating when the radius of curvature at the peak and valley reaches a critical radius $|R^*_{\text{crit}}| = 1/\Delta F^*$. Thereafter, the boundary shape no longer changes (i.e., an equilibrium shape is reached) and can be calculated by a closed-form solution to the kinetic equation governing grain boundary migration. Nevertheless, when $\Delta F^* > 2\pi$, the equilibrium solution does not exist and the boundary migrates indefinitely, becoming elongated and never reaching an equilibrium shape. The radius of curvature at the peak and valley decreases down to $1/2\pi$, regardless of the $\Delta F^*$ value, never reaching the critical radius. This result is unexpected and might be related to the mechanism of grain boundary migration that leads to the GDRX.

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