Static recrystallization study on pure aluminium using crystal plasticity finite element and phase-field modelling

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Abstract

In-depth understanding of the recrystallization process in alloys is critical for generating desirable small grains and weak textured microstructure, which provides high strength and toughness for metal formed parts. The manufacturing industry has a high demand for a valid computational model to accurately predict the level of recrystallization and recrystallized grain size under different strain paths and temperatures. However, current understanding and numerical calculation have not been linked properly for a reliable, physically based model to simulate the deformation and annealing process. Our phase-field model coupled with crystal plasticity simulations, which is based on the theory of stored energy minimization, enables a reliable prediction on the microstructure evolution under different processing routes. We hope that this modelling work provides a solution for the prediction of some long standing microstructure formation problems.

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Keywords: Static recrystallization; Phase-field model; Crystal plastic finite element model; Pure aluminium

1. Introduction

Recrystallization is demonstrated to be a powerful way to produce the desired microstructure through the material manufacturing processes. Hence, a reliable computational model of recrystallization based on sound physical concepts...
is vital to optimize the microstructure and obtain specific material properties for alloys used in aeroplane [1, 2]. The optimal processing parameters during the manufacture, such as deformation magnitude, processing temperature and processing time, are aimed to be determined at a grain-scale through the computational simulation [3].

The term, recrystallization, was defined by Doherty, Gottstein, Hirsch et al. in 1988 as “the formation of a new grain structure in a deformed material by the formation and migration of high angle grain boundaries driven by the stored energy of deformation” [4]. The driving force for the boundary migration is from the stored energy reduction and minimization of surface energy [5].

The phase-field model proposed by Kobayashi, Warren and Carter [6] is used in this paper to study the grain growth phenomenon. It has two order variables, the phase-field \( \phi \) and crystal orientation \( \theta \). The microstructure study for recrystallization typically consists of a number of grains represented by the two variables of the phase-field model [7]. Within the grain, the phase-field model variables have nearly constant values which are associated with grain orientation and structure. At interface between grains, the variables gradually vary over a narrow region between their values in neighboring grains [8]. It is known as diffuse-interface approach which allows us to predict the evolution of arbitrary complex morphologies without making any presumptions on the shape of grain [5]. For the recrystallization process, microstructure evolution is comprised of the nucleation and growth of new grains at particular sites [9]. Nucleation is usually incorporated into simulations using separate analytical models. It is not feasible to consider the nucleation and grain growth at the same time from a view of computational effort, as an extremely small resolution and time step over the whole domain is required to catch the nucleation phenomenon [8].

In this paper, a phase-field model together with a crystal plasticity finite element method is applied to study the microstructure evolution of static recrystallization during annealing [10, 11]. The combined model is able to predict the recrystallization process for grain size distribution and recrystallization fraction evolution of alloy under certain processing routes.

## 2. Methodology

### 2.1. Crystal plasticity finite element model

The crystal plasticity finite element model used in this project is rate-sensitive and implemented in the user material subroutine using Abaqus standard/explicit analysis. The total deformation gradient, \( F \), consists of elastic deformation gradient, \( F^e \), and plastic deformation gradient, \( F^p \), as shown in Eq. (1).

\[
F = F^e F^p, \tag{1}
\]

\( F^e \) is determined from anisotropic Hooke’s law and \( D^p \) is determined from the plastic velocity gradient \( L^p \), using \( D^p = \text{sym}(L^p) \). The \( L^p \) in terms of the summation of the contributions from all active slip systems in turn is given by

\[
L^p = \hat{F}^p F^p^{-1} = \sum_{\alpha=1}^{12} \gamma^\alpha s^\alpha \otimes n^\alpha, \tag{2}
\]

where \( s^\alpha \) is the line vector along slip direction and \( n^\alpha \) is the slip plane normal of slip system \( \alpha \). The rate of dilocation slip, \( \dot{\gamma}^\alpha \), on the slip system \( \alpha \) is given by

\[
\dot{\gamma}^\alpha = \rho^\alpha_{\text{SSD}} b \gamma \exp\left(-\frac{\Delta H}{kT}\right)\sinh\left(\frac{\Delta V}{kT}\right)\left|\tau^\alpha - \tau_c^\alpha\right|, \tag{3}
\]

where \( \rho^\alpha_{\text{SSD}} \) is the gliding dislocation density, \( b \) is the magnitude of Burgers vector, \( \gamma \) is the jump frequency for driving thermally activated dislocation escape, \( \Delta H \) is the Helmholtz free energy, \( \Delta V \) is the associated activation volume, \( \tau^\alpha \) is the resolved shear stress and \( \tau_c^\alpha \) is the critical resolved shear stress of the slip system \( \alpha \). Hence, the accumulated slip on the slip system \( \alpha \), \( \gamma^\alpha_{t+\Delta t} \), after a certain period, \( \Delta t \) is expressed as

\[
\gamma^\alpha_{t+\Delta t} = \gamma^\alpha_t + \int_t^{t+\Delta t} \dot{\gamma}^\alpha dt = \gamma^\alpha_t + \left[\gamma^\alpha_{t+\Delta t}\right] \Delta t, \tag{4}
\]

For modelling the plastic behaviour, a modified Taylor hardening rule used to describe the isotropic hardening is given by

\[
\tau_c^\alpha = \tau_c^{\alpha_0} + \mu \cdot G_{12} \cdot b \cdot \sqrt{\rho_{\text{GND}} + \rho_{\text{SSD}}}, \tag{5}
\]
where \( \tau_{c0}^{\alpha} \) is the initial slip strength, \( \mu \) is a constant from literature for pure aluminium, \( G_{12} \) is the shear modulus, \( \rho_{\text{GND}} \) is the geometrically necessary dislocation density and \( \rho_{\text{SSD}} \) is the sessile statistically stored density. The evolution of SSD density has linear relationship with accumulated slip rate as
\[
\rho_{\text{SSD}} = \lambda \cdot \dot{\rho},
\]
where \( \lambda \) is the hardening coefficient, and the effective plastic strain rate \( \dot{\rho} \) is expressed by
\[
\dot{\rho} = \left( \frac{2}{3} \mathbf{L}^p : \mathbf{L}^p \right)^{\frac{1}{2}},
\]
Nye’s dislocation tensor using to compute the components of geometrically necessary dislocation density is given by
\[
\Lambda = \text{curl} \left( \mathbf{F}^p \right) = \sum_{\alpha=1}^{12} \rho_{\text{Gos}}^\alpha \mathbf{b}^\alpha \otimes \mathbf{s}^\alpha + \rho_{\text{Gen}}^\alpha \mathbf{b}^\alpha \otimes \mathbf{t}^\alpha + \rho_{\text{Gen}}^\alpha \mathbf{b}^\alpha \otimes \mathbf{n}^\alpha,
\]
where \( \rho_{\text{Gos}}^\alpha \) are the screw dislocation components on slip system \( \alpha \) with line vector along the slip direction \( \mathbf{s}^\alpha \), \( \rho_{\text{Gos}}^\alpha \) and \( \rho_{\text{Gen}}^\alpha \) are the edge dislocation components with line tangent vector along the slip normal \( \mathbf{n}^\alpha \) and \( \mathbf{t}^\alpha \) respectively, \( \mathbf{t}^\alpha = \mathbf{s}^\alpha \times \mathbf{n}^\alpha \) and \( \mathbf{b}^\alpha \) is the Burgers vector on slip system \( \alpha \).

The 36 independent geometrically necessary dislocation density components, that include 12 \( \rho_{\text{Gos}}^\alpha \)crew, 12 \( \rho_{\text{Gen}}^\alpha \)edge and 12 \( \rho_{\text{Gen}}^\alpha \)edge dislocation components, need to be solved from the equations listed above. Eq. (8) may be written in a matrix as
\[
\Lambda = \mathbf{A} \rho_{\text{GND}},
\]
where \( \mathbf{A} \) is a 9×1 vector form of the Nye’s dislocation tensor \( \Lambda \), \( \mathbf{A} \) is a 9×36 linear matrix containing the basis tensors \( \mathbf{b}^\alpha \otimes \mathbf{s}^\alpha \), \( \mathbf{b}^\alpha \otimes \mathbf{t}^\alpha \) and \( \mathbf{b}^\alpha \otimes \mathbf{n}^\alpha \). The sum of squares of geometrically necessary dislocation densities on each slip is expressed as:
\[
\rho_{\text{GND}} = \sqrt{\rho_{\text{Gos}}^2 + \rho_{\text{Gen}}^2 + \rho_{\text{Gen}}^2}.
\]

The parameters used in crystal plasticity finite element model to simulate the plastic deformation of pure aluminium at room temperature are listed in Table 1. Only the initial slip stress \( \tau_c \) for yield point determination and isotropic hardening coefficient \( \lambda \) in Eqs. (4), (5) and (6) were determined through seeking best agreement with uniaxial tensile curve, whereas the other properties, like Young’s Modulus \( E \), shear Modulus \( G_{12} \), Burgers vector magnitude \( b \), Boltzmann constant \( k \), Helmholtz free energy \( \Delta H \) and activation volume \( \Delta V \) were chosen from literature for pure aluminium [12, 13]. The \( \Delta H \) in this study neglected the strain rate sensitivity of stress behaviour of pure aluminium alloy at room temperature.

<table>
<thead>
<tr>
<th>( \rho_{\text{SSD}} ) (( \mu m^{-2} ))</th>
<th>( b ) (( \mu m ))</th>
<th>( v ) (( s^{-1} ))</th>
<th>( \Delta H ) (( J ))</th>
<th>( k ) (( \mu m^{-2} ))</th>
<th>( \tau_c ) (( \mu m^{-2} ))</th>
<th>( \lambda ) (( \mu m^{-2} ))</th>
<th>( \mu )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>2.86×10^{-4}</td>
<td>1×10^{11}</td>
<td>2.9×10^{-20}</td>
<td>1.381×10^{-21}</td>
<td>0.1</td>
<td>0.1</td>
<td>0.22</td>
</tr>
</tbody>
</table>

### 2.2. Phase-field model
In this model, the grain boundary migration during the recrystallization is driven by the stored energy which is a generalisation of phase-field model [14]. Two order variables are applied: one is phase-field variable \( \varphi \), taking a value of 0 for deformed grains and 1 for recrystallized grains; the other one is the crystal orientation \( \theta \) of the recrystallized grain. To simplify the calculations for phase-field model, only the z-axis orientation of the crystal is chosen to represent the crystal orientation in this study.

The free energy function using the order variable \( \varphi \) and \( \theta \) is expressed by...
\[ F = \int \left[ \frac{\alpha^2}{2} |\nabla \varphi|^2 + f_d(\varphi) + f_e(\varphi + \rho) + g(\varphi) s |\nabla \theta| \right] dV. \] (11)

The time evolution equations for \( \phi \) and \( \theta \) are calculated as
\[ \dot{\phi} = M_\phi \left[ \alpha^2 \nabla^2 \phi - \frac{\partial f_d}{\partial \phi} - \frac{\partial f_e}{\partial \phi} - \frac{\partial g}{\partial \phi} s |\nabla \theta| \right], \] (12)
\[ \dot{\theta} = M_\theta \frac{1}{\phi^2} \left[ g(\phi) s \frac{|\nabla \theta|}{\nabla \theta} \right]. \] (13)

The variables in above equations are expressed as following:
\[ f_d(\varphi) = W q(\varphi), \] (14)
\[ q(\varphi) = \varphi^2 (1-\varphi)^2, \] (15)
\[ f_e(\varphi, \rho) = f'_e(\rho) p(\varphi) + f''_e(\rho)(1-p(\varphi)), \] (16)
where \( f_d(\varphi, \rho) \) is the stored energy density, \( f'_e(\rho) p(\varphi) \) and \( f''_e(\rho)(1-p(\varphi)) \) are the stored energy densities in the recrystallized grains and deformed grains. \( f'_e(\rho) = 0 \) and \( f''_e(\rho) = 20 \times E_{store} \) have been chosen.

The stored energy per unit length of a deformed alloy \( E_{store} \), which is related with the dislocation density \( \rho \), is expressed by
\[ E_{store} = 0.5 \rho G_1 b^2. \] (17)
\[ p(\varphi) \] is a interpolating function to smooth the density inside the interface region and is expressed by
\[ p(\varphi) = \varphi^3 (10-15\varphi + 6\varphi^2). \] (18)
\[ g(\varphi) \] used to eliminate the effect of misorientation inside the deformed grain is given by
\[ g(\varphi) = \varphi^2. \] (19)

The gradient coefficient \( \alpha \) and the barrier height \( W \) are associated with grain boundary thickness \( \delta \) and grain boundary energy \( \sigma \).
\[ \alpha = \sqrt{\frac{3\delta \sigma}{a}}, \] (20)
\[ W = \frac{6\sigma a}{\delta}. \] (21)
\[ a = 2.20 \] if the interface region is \( \varphi = [0.1, 0.9]. \) (22)
\[ \delta = 4\Delta x. \] (22)
\[ \Delta x \] is the grid size.

\( M_\phi \) and \( M_\theta \) are the mobilities of \( \phi \) and \( \theta \). The grain boundary mobility \( M \) is given by
\[ M = M_\phi \exp(-\frac{Q}{RT}) = M_\theta \exp(-\frac{Q'}{k_B T}). \] (23)

\( M_0 \) is a pre-exponential factor, \( Q \) and \( Q' \) are activation energies, \( R \) is the gas constant, \( T \) is the annealing temperature and \( k_B \) is the Boltzmann constant.

The rotation of grains are restricted by setting
\[ M_\theta = (1-p(\varphi))M''_\theta, \] (24)
\[ M'_\theta = M_\phi, \] (25)
\[ s = \frac{\alpha \sqrt{2W}}{\pi}. \] (26)

The nucleation of recrystallised grains is simulated based on the seeding criteria in the results part. The grain growth driven by the stored energy follows the time-evolution equations of the two order parameters \( \varphi \) and \( \theta \), i.e. Eqs. (12) and (13). The 2D map is solved using finite difference and the Euler Forward method is used for the time integration.

The parameters used in phase-field model to simulate the static recrystallization at 800 K are listed in Table 2.
Table 2. Material parameters for phase-field model.

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>$\sigma$</th>
<th>$T$</th>
<th>$k_B$</th>
<th>$M_0$</th>
<th>$Q^*$</th>
<th>$\Delta t$</th>
<th>$\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\mu m))</td>
<td>(J/m(^2))</td>
<td>(K)</td>
<td>(J/K)</td>
<td>(J)</td>
<td>(J)</td>
<td>(s)</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.6</td>
<td>800</td>
<td>$1.38 \times 10^{-23}$</td>
<td>$6.2 \times 10^{-6}$</td>
<td>$2.08 \times 10^{-19}$</td>
<td>0.01</td>
<td>2.20</td>
</tr>
</tbody>
</table>

3. Results and discussion

3.1. Crystal plasticity finite element model

3D crystal plasticity modelling was applied to investigate the behaviour of polycrystalline pure aluminium, whereas only the middle XY layer of the model was extracted and input to the phase-field model to simulate the recrystallization behaviour.

Twenty-noded brick finite elements with reduced integration were used. All results were extracted from integral points on the free front surface of the model with spacing of $6 \mu m$. The finite element model comprised 49 grains with random orientations generated by VGRAIN [15] with 4 elements through the depth of sample shown as Fig. 1(a) and (b). The reason to put 4 elements on Z-axes is that the geometrically necessary dislocation density distribution calculated from 3D crystal plasticity model is more close to the real deformed microstructure which has been verified by electron back-scattered diffraction technique. The model was deformed to 5% uniaxial compression strainning at room temperature. The bottom, left and back surface were fixed as the boundary conditions of the model. Hence, comparisons are feasible between the experimental observations and modelling results.

The polycrystal pure aluminium model measured the area of $210 \times 210 \times 30 \mu m^3$ with average grain diameter 30 \(\mu m\). Pole figure to describe the polycrystal pure aluminium model with no texture is shown in Fig. 1(c). The developed crystal plasticity model was calibrated to match the experimental macroscopic stress strain response of polycrystalline pure aluminium without texture. The simulated stress strain curve together with experimental curve under uniaxial tensile test are shown in Fig. 1(d) using the slip rule parameters in Table 1.

The dislocation and grain orientation distribution on the middle XY layer in Z axis was extracted from the crystal plasticity finite element model together with the displacement information of grid to maintain the deformed shape. These data was imported into the phase-field model to simulate the recrystallization after the data smoothing. The dislocation density distribution simulated by crystal plasticity model is an important parameter to predict the exact position of possible nucleation points and the grain growth rate during annealing. This simulated dislocation distribution can be verified through making a comparison with the geometrically necessary dislocation distribution of an electron back-scattered diffraction map according to the intragranular misorientation calculation.

3.2. Data mapping

The crystal orientation and dislocation density from the crystal plasticity analysis were used as the input information for phase-field model to calculate grain nucleation and grain growth during the recrystallization. Due to the difference in grid size and element shape, the data from crystal plasticity finite element model was remapped through linear interpolation [16] (see Fig. 2), as the driving force required for phase-field model needs to be distributed smoothly inside the interface region.
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<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta x$ (μm)</td>
<td>1800</td>
</tr>
<tr>
<td>$\sigma$ (2J/m²)</td>
<td>1807</td>
</tr>
<tr>
<td>$T$ (K)</td>
<td>1805</td>
</tr>
<tr>
<td>$B_k$ (J/K)</td>
<td>1800</td>
</tr>
<tr>
<td>$M$ (J/K)</td>
<td>1804</td>
</tr>
<tr>
<td>$Q$ (J)</td>
<td>1803</td>
</tr>
<tr>
<td>$\Delta t$ (s)</td>
<td>1802</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>1801</td>
</tr>
<tr>
<td>$\beta$</td>
<td>1800</td>
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3.3. Grain nucleation

The nucleated grains were added manually to the microstructure based on the seeding criteria. The mechanisms of grain nucleation have been clarified [1]: i) high angle grain boundary is necessary; ii) high stored energy is necessary; iii) new orientations of nuclei are present in the deformed grain structure. Hence, the seeding criteria for the nuclei require a critical stored energy $E_c$ and a misorientation $\Delta \theta$ at the grit point, which means only the grit points with...
high stored energy located at the high angle grain boundary can be seeded as the nuclei of new grains. The high angle grain boundary was set to be more than 10° in this paper; the $E_c$ was assumed to be 1 MPa per unit length and the orientations of nuclei were set to be a random orientation. In addition to the above conditions, the distance between two neighboring nuclei was set to be more than 10 μm and the nuclei size was set to be 4 μm. The reason to assume the site-saturated nucleation model is because the phase-field method uses the diffusive interface region with a finite width [10]. The dislocation density distribution $\rho$, phase distribution $\phi$ and theta distribution $\theta$ in the range of $[0, \pi]$ after seeding are shown in Fig. 3. The orientation of $\theta$ is measured in radians.

**3.4. Grain growth**

The grain growth driven by the reduction of dislocation energy, interfacial energy and curvature energy was simulated by the phase-field model and shown in the Fig. 4. The nuclei having no dislocation density and random crystal orientation generated on the grain boundaries grew gradually into grains with high dislocation energy during time evolution, and finally wiped out the deformed grains after enough annealing time. New grain boundaries were formed during recrystallization. The evolution of grain size and recrystallized fraction can be extracted from Fig.4, and then calibrated with Johnson-Mehl-Avrami-Kolmogorow curve and/or experimental results.

![Fig. 3](image1.png)

**Fig. 3.** (a)-(c) shows information of dislocation density $\rho$, phase $\phi$ and crystal orientation $\theta$ after seeding nucleation sites.

![Fig. 4](image2.png)

**Fig. 4.** (a)-(b) shows change of two order parameters $\phi$ and $\theta$ respectively through phase-field simulation for static recrystallization process after $0\ s$, $1\times10^3\ s$, $1\times10^5\ s$ and $5\times10^5\ s$ annealing.

In Fig. 4, the deformed material was completely recrystallized after a sufficiently long period time, e.g. $10^6\ s$, which demonstrates that this numerical method on the basis of the deformed microstructure calculated by crystal
plasticity model is able to simulate the recrystallization microstructure changes including the new grain nucleation and grain growth during annealing. However, the defined criteria of the phase-field model, such as the size and orientation of nuclei, the dislocation density distribution on the deformed material, and the grain growth rate, were not calibrated with the experimental results. Electron back-scattered diffraction technique can be used in the future to verify the geometrically necessary dislocation distribution, the orientation of nuclei and its grain growth rate. Furthermore, the nucleation and grain growth simulations were separated in this study which is not true in reality and needs to be improved. The nucleation should occur spontaneously anytime during annealing once the criteria are reached.

4. Conclusions

A phase-field model coupled with crystal plasticity finite element model has been established in this paper to simulate the static recrystallization behavior of a deformed pure aluminium. Data mapping has been applied to the crystal plasticity finite element calculated data that have irregular size and shape of finite elements to achieve smoothly distributed driving forces for phase-field model. The nucleation and grain growth of recrystallization are separated in this phase-field model through defining the nucleation criteria and grain growth kinetics independently. This phase-field model enables the simulation of recrystallization process including the grain nucleation and grain boundary migration during annealing.

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