3D microstructural evolution of primary recrystallization and grain growth in cold rolled single-phase aluminum alloys

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Abstract

Modeling the microstructural evolution during recrystallization is a powerful tool for the profound understanding of alloy behavior and for use in optimizing engineering properties through annealing. In particular, the mechanical properties of metallic alloys are highly dependent upon evolved microstructure and texture from the softening process. In the present work, a Monte Carlo (MC) Potts model was used to model the primary recrystallization and grain growth in cold rolled single-phase Al alloy. The microstructural representation of two kinds of dislocation densities, statistically stored dislocations and geometrically necessary dislocations were quantified based on the ViscoPlastic Fast Fourier transform method. This representation was then introduced into the MC Potts model to identify the favorable sites for nucleation where orientation gradients and entanglements of dislocations are high. Additionally, in situ observations of non-isothermal microstructure evolution for single-phase aluminum alloy 1100 were made to validate the simulation. The influence of the texture inhomogeneity is analyzed from a theoretical point of view using an orientation distribution function for deformed and evolved texture.

Keywords: dislocation density, Monte Carlo Potts model, recrystallization, rolled single-phase Al alloy, in situ annealing, texture, VP-FFT
1. Introduction

Modeling microstructural evolution has become an indispensable tool for many metals processing companies because the alloys can first be designed computationally by tailoring their microstructural features [1, 2]. These features entail grain size, particle/precipitate content, recrystallization fraction, and crystallographic texture, among others [3]. Additionally, given the complication of industrial thermo-mechanical processes, various annealing phenomena, such as recrystallization and grain growth, are incompletely understood. Because of this, many efforts have focused on the development of computer simulations for recrystallization and grain growth [4]. Among the computer simulation methods is the Monte Carlo (MC) Potts model. This model has been used to simulate annealing phenomena such as grain growth in single- and two-phase polycrystalline materials [5–7], directional grain growth [8], particle pinning [9], static recrystallization [10], dynamic recrystallization [11], microstructure evolution in the presence of anisotropy [12], abnormal grain growth [13], nanocrystalline grain growth [14], and particle stimulated nucleation dominated recrystallization [15]. The MC Potts method has also demonstrated its applicability to modeling recrystallization in aluminum alloys [16].

In general, coupling two computational methods to predict the microstructural evolution starting with a deformed structure obtained from another model has been investigated in the past. For example, Radhakrishnan et al [17] have coupled the finite element crystal plasticity method with MC Potts model to simulate recrystallization in a particle containing alloy. Lee et al [18] have integrated a phase field model with ViscoPlastic Fast Fourier transformation (VP-FFT) method to simulate recrystallization. None of these attempts have explicitly considered the microstructural representation of recrystallization driving force distributions as favorable sites for growth of subgrains that become recrystallization nuclei. In the current study, the two dislocation densities (statistically stored dislocations (SSDs) and geometrically necessary dislocations (GNDs)) are formulated based on a VP-FFT method [19]. The SSD densities are formulated to quantify the heterogeneous distribution of the recrystallization driving force due to the tangling and trapping of dislocations during crystallographic slip on different slip planes [20, 21]. Whereas, GNDs are formulated to identify orientation gradients in the microstructure due to plastic deformation [20, 21].

The arrangement of these dislocation densities is mechanically stable in a deformed matrix [22, 23]. On the other hand, they are not thermodynamically stable, but rather become the favorable places for strain-free grains to nucleate within the deformed matrix when it is subjected to temperatures on the order of 0.4 $T_m$ [24]. For most commercial aluminum alloys, it has experimentally been demonstrated that nucleation takes place at grain boundaries, where the misorientation and stored energy gradients are high [25]. This non-random distribution may have a considerable impact on both the size distribution of recrystallized grains and the kinetics of recrystallization [26, 27]. Hence, in the present simulation every voxel of the digital structure was assigned a scalar value corresponding to the total dislocations (SSDs and GNDs), which contributes to the total energy of the system, and the recrystallizing subgrains that have preferentially been introduced at positions of high SSDs and GNDs [28].

An understanding of recrystallization textures is of industrial importance since the texture is responsible for the anisotropy in mechanical properties of the material, and will, in many cases, determine the properties of the product [25, 29, 30]. These properties will depend on
whether the grains are randomly oriented or tend to have preferred crystallographic orientation [30]. Orientation changes occur due to sliding on the most favorably oriented slip or twinning systems during deformation [25]. To represent textures appropriately, special techniques are needed to describe the orientation alterations that occur during deformation separately from the microstructural development. Orientation distribution functions (ODF) are adopted to provide a comprehensive description of deformed and developed textures [31]. The orientations (i.e. texture) of the digital microstructures are matched to common texture components that are found in rolling textures of FCC metals in addition to considerable fractions of other components [4, 22, 31]. The initial deformed texture of the digital microstructure will be changed during recrystallization and grain growth to common preferred orientations for recrystallization texture. The initial microstructure was statistically formed using the Dream3D software [32], and the initial as well as the evolved orientation textures were visualized by MTEX software [33]. The main purpose of the present work is to implement the computer simulation to properly predict the microstructural evolution during primary recrystallization of a single-phase aluminum alloy. The dislocation density distributions (SSDs and GNDs) were formulated based on the VP-FFT method, then, the spatial distribution of these dislocation densities was coupled to the MC Potts model to characterize the nucleation locations. The quantitative analysis of the evolved structures was performed on two parameters, namely the average grain size and the fraction of recrystallized grains. Additionally, non-isothermal annealing microstructure evolution for single-phase aluminum alloys is also determined to validate the simulation behavior.

2. Simulation approach

2.1. VP-FFT method

The VP-FFT method that sometimes is referred to as extended-VPSC is based on the influential work of Molinari et al [34]. This formulation (VPSC) has been developed to account for polycrystalline aggregates and to clarify the experimental deformation phenomenon on metallic and geological materials [35]. The conventional n-site VPSC method is not generally used with complex and large-scale microstructures (due to extensive computational requirements, even in the simplified case of considering only first-neighbor interactions). Thus, the VP-FFT was developed to overcome the downside of the n-site self-consistent formulation. For further explanations the reader is referred to Lebensohn (2001) [36]. In the current simulations, the polycrystalline structure is modeled initially by 430 grains with typical rolling texture orientations in the un-deformed state. The VP-FFT method has been used to determine the overall and local mechanical response of the 3D rolled structure of a pure Al alloy, using the following imposed velocity gradient [19, 37]:

$$\vec{L}_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

which assumes plane strain deformation. The basic concept of the VP-FFT describes the interaction between a grain, as an inclusion, and the homogeneous effective medium that accommodates the inclusion (grain) to solve the equilibrium equation. The Green’s functions present the unknown components of the velocity gradient and the strain rate fields as convolutions in the real space, which in turn are stated as a tensor product in the Fourier space. Afterwards, the FFT determines the strain rate field [38]. The local constitutive equation (power law relationship) for stress and strain rate for every Fourier point are solved
in an iterative way \[19, 39\]
\[
\dot{\varepsilon}(s) = \tau_o \sum_s m^s \left( \frac{m^s \sigma^s(\tau)}{\tau_o} \right)^n,
\]
where \(m^s = \frac{1}{2}(n^s b^s + n^s b^s)\) is the Schmid tensor for a particular slip system \(s\), where \(n^s\) and \(b^s\) are the normal and Burgers vector of such slip (or twinning) system, \(\tau^s_o(x)\) is the threshold resolved shear stress, \(\dot{\gamma}_o\) is a normalization factor, and \(n\) is the rate-sensitivity exponent, which is usually set to 20 such that the texture development is in the rate-insensitive regime \[19\]. The updated deviatoric stress tensor \(\sigma^s(\tau)\) is utilized for computing the stress field. In our polycrystalline simulations, the empirical extended Voce law to describe the variation of \(\tau^s\) in each system of each deformation mode was used \[40\]. This formula characterizes the evolution of the threshold stress with accumulated shear strain in each grain. The evolution of the slip resistance for each slip system, \(s\), is given by
\[
\dot{\tau}^s = \tau^s_o + (\tau^s_0 + \theta^s_0 \Gamma) \left( 1 - \exp \left( -\Gamma \frac{\theta^s_0}{\tau^s_0} \right) \right),
\]
where \(\Gamma\) is the accumulated shear in a grain and \(\tau^s_0, \theta^s_0, \theta^s_1, \text{ and } (\tau^s_0 + \tau^s_1)\) are the initial threshold stress, the initial hardening rate, the asymptotic hardening rate, and the back-extrapolated threshold stress, respectively \[19\]. The increase in threshold stress in each slip system can be described, after a time increment \(\Delta t\), in terms of coupling coefficients \(h^s\) of self and latent hardening and \(\dot{\gamma}^s\) the local shear-rate on slip system \(s\), \[19\]
\[
\Delta \tau^s = \frac{d\tau^s}{dt} \sum_{s'} h^s_{s's'} \Delta t.
\]

2.2. Dislocation density

Generally, the strengthening of polycrystalline metals is gained due to the existence of dislocations: statistically-stored dislocations (redundant), which evolve due to random trapping processes through the plastic deformation, and geometrically necessary dislocations (non-redundant), which appear in orientation gradient fields for geometrical compatibility within the crystal lattice \[21\]. These two forms of dislocations together comprise the total dislocation density \(\rho_{\text{total}} = \rho_{\text{stat}} + \rho_{\text{geo}}\) as a scalar quantity characterizing the driving force for recrystallization (stored energy). On the other hand, these two dislocation types are not introduced in the constitutive laws of VP-FFT. They are quantified implicitly based on VP-FFT calculations (local shearing stresses and local velocity gradients for every active slip system in the crystal lattice in the grain) only to identify the favorable sites of nucleation where orientation gradients and entanglements of dislocations are high \[21\]:
\[
H(s_t) = \rho_{\text{total}}(s_t).
\]

2.2.1. Statistically stored dislocations. The SSDs can be related to the slip resistance. They are present in the form of tangles, dipoles and multipoles, which yields an effective density for SSDs on a slip system \(s\). Taylor \[41\] has shown that the slip resistance as a result of dislocation interactions can be measured as the square root of the average dislocation density,
\[ \rho_{\text{gnd}}^s = \left( \frac{\tau^s}{\alpha \mu b} \right)^2, \]  

where \( \alpha \) is a constant on the order of 0.5, \( \mu = 25.4 \) GPa is the shear modulus, \( b \) is the Burgers vector with a magnitude of 0.286 nm \([42]\), and \( \tau^s \) is the accumulated shear stress that is defined with the Voce law (the constitutive relation of strain hardening that controls the VP-FFT model) \([43]\).

### 2.2.2. Geometrically necessary dislocations

The presence of GNDs at a deformed structure is necessary in order to maintain lattice compatibility by supporting a curvature in the crystallographic lattice \([44]\). The notion of GNDs was first presented by Nye \([45]\) quantifying the dislocation content in the lattice by Nye’s dislocation density tensor, \( \alpha_{ij} \). Sun et al have shown that Nye’s original formulation of the dislocation density tensor can be retrieved from the fundamental equation of continuum dislocation theory, equation (6), that relates the dislocation tensor to the elastic strain and curvature of the crystallite lattice in the absence of long-range elastic stress fields \([46]\)

\[ \alpha_{ij} = \epsilon_{ijkl} (\epsilon_{ijkl} + g_{ijkl}), \]  

\[ \alpha_{ij} = \epsilon_{ijkl} g_{ijkl}. \]  

Nye’s tensor can also be formulated in terms of the velocity gradient that is extracted from the VP-FFT results \([47]\)

\[ \dot{\alpha}_{ij} \equiv \epsilon_{ijkl} L_{ijkl}^p. \]  

El-Dasher et al \([48]\) have shown that the norm of \( \alpha_{ij} \) is proportional to the geometrically necessary bulk dislocation density in an FCC material. It holds that:

\[ \rho_{\text{gnd}}^s = \frac{1}{b} \sqrt{\alpha_{ij} \alpha_{ij}}. \]  

Here \( \alpha_{ij} = 0 \) implies the absence of GNDs \([49]\), where \( \epsilon_{ijkl} \) are components of the permutation tensor, \( \epsilon_{ijkl} \) is the infinitesimal elastic strain gradient, and \( g_{ijkl} \) is the gradient in lattice orientation, where \( i \) is the time and \( L^p \) is the velocity gradient, which is the sum of shearing rates from every active slip system in the crystallite lattice, and \( b \) is the Burgers vector for aluminum on the order of 2.86 nm (see \([50]\)).

### 2.3. Potts model

To perform MC Potts model simulations, a 3D digital microstructure is mapped onto a cubic lattice by apportionment of each lattice site \( i \), a spin \( S_i \), which corresponds to a crystallographic orientation. The number of grains in this initial structure is 430; every voxel \((128 \times 128 \times 128 = 2097152 = N)\) was assigned an orientation index \( S_i \leq 430 \). The grain boundaries are considered as the lattice sites which are surrounded by sites having different orientations \([19]\). The total simulation time of recrystallization and grain growth was 300 MC Steps.
The entire system’s energy is designated by the Hamiltonian equation below,

\[ E = \sum_{i=1}^{N} \sum_{j=1}^{N} \gamma(S_i, S_j) + \sum_{i=1}^{N} H(S_i), \]  

where every site contributes to the bulk energy of the system, \( H(S_i) \). For the initially unrecrystallized matrix, \( H(S_i) \) was set to the total dislocation density (the sum of the statistically stored and geometrically necessary densities) and zero for recrystallized material. The external summation in the Hamiltonian, equation (11), is over all \( N \) sites in the system. The internal summation is over the nearest neighbors of the chosen site or spin. \( S_i \) and \( S_j \) are old and new (randomly selected) spins, respectively.

One Monte Carlo time step (MCS) represents \( N \) reorientations for the whole system, where each of the \( N \) sites is given an opportunity to change orientation. The Read–Shockley formula was applied to represent the grain boundary energy variation at small misorientations less than 15° along with an exponential variation of mobility \([51, 52]\). An orientation identifier for each lattice site was introduced for incorporating the crystallographic anisotropy in the MC approach. Hence, each lattice site was allocated with both a spin identifier, \( S_i \), and an orientation identifier (three Euler angles).

The normalized expression for the grain boundary energy as a function of misorientation is used in the present implementation of the MC Potts model:

\[ \gamma = \gamma_0 \frac{\theta}{\theta_m} \left\{ 1 - \ln \left( \frac{\theta}{\theta_m} \right) \right\}, \]  

where \( \theta_m \) is the maximum misorientation angle of low angle grain boundaries. It has been reported that \( \theta_m \) lies within 10°...30° \([52]\). In this work \( \theta_m \) was set to 15°. It follows:

\[ J(S_i, S_j) = \begin{cases} 0 & \text{in the grain interior } (S_i = S_j) \\ \frac{\gamma}{2} & \text{for the boundaries } (S_i \neq S_j). \end{cases} \]  

The mobility of grain boundaries is a function of misorientation as well. Equation (14) defines the mobility between two adjacent spins, \( S_i \) and \( S_j \), where the orientation identifiers indicate the Euler angles of the lattice sites \([19]\):

\[ M(S_i, S_j) = 1 - \exp \left\{ -5 \left( \frac{\theta}{\theta_m} \right)^4 \right\}. \]  

The site saturated surface nucleation and oriented nuclei were used in this work. The orientation values were arranged into recrystallized and unrecrystallized sets of spins. The evolution of the structure itself is simulated by choosing a spin from the unrecrystallized orientation and flipping it by a new orientation chosen randomly from the set of allowable values for recrystallization \([29]\). The change in the total system energy, \( \Delta E \), for re-flipping the spin of the site to the nominee spin is calculated by equation (10), and reorientation of spins were executed with transition probability \( P \) according to:

\[ P(S_i, S_j, \Delta E, T) = \begin{cases} \frac{J(S_i, S_j) M(S_i, S_j)}{J_{\text{max}} M_{\text{max}}} \Delta E \leq 0 \\ \frac{J(S_i, S_j) M(S_i, S_j)}{J_{\text{max}} M_{\text{max}}} \exp \left\{ \frac{-\Delta E}{kT} \right\} \Delta E > 0, \end{cases} \]

\([14]\)
where $J_{\text{max}}$ and $M_{\text{max}}$ are the maximum boundary energy and mobility in the system respectively [15, 33]. In the current simulation, we use $J_{\text{max}} = 1$ and $M_{\text{max}} = 1$. To retain boundary roughness and evade lattice pinning the lattice temperature $(kT)$ was set to 0.2–0.3 so as (compare [53, 54]).

3. Results and discussion

3.1. Experimental in situ microstructural evolution

In situ thermal annealing has been carried out experimentally using electron backscatter diffraction to present static recrystallization behavior in cold rolled 70% reduction of an 1100 aluminum alloy. Figures 1(a)–(c) show the IQ image, orientation map, and kernel average misorientation (KAM) map for the cold rolled AA1100 at room temperature, respectively.
In particular, in figure 1(a), the white arrows point to the regions near the triple junctions and grain boundaries that are packed with pre-existing subgrains with partial high angle boundaries. These regions are clearly condensed with stored energy (SSDs) and orientation gradient (GNDs) as indicated by the white arrows, figures 1(b) and (c). In addition, in figure 1(c) the dark regions in the KAM map designate the high misorientation regions, which reflect the GND distribution in the microstructure. As in situ annealing continues it can be noted that recrystallizing subgrains grow and some vanish and are replaced with other subgrains nucleated just below the surface, figures 1(d)–(f). These developments in the recrystallized microstructures confirm that nucleation and growth of the recrystallized grains have heterogeneous character near the grain boundaries giving rise to the fast recrystallization at the subgrains along the grain boundaries parallel to the rolling direction, which matches the simulation results below. The recrystallizing grain size increases with increasing temperature from 250 °C to 350 °C, however, only relatively slowly as can be observed in figures 1(d)–(i).

3.2. Dislocation spatial distribution

To properly model recrystallization, the dislocation density and its spatial distribution in the microstructure are a necessity to be quantified correctly. This is not only because the dislocations act as the driving pressure for recrystallization but also because the heterogeneous distribution of the dislocations identifies precisely the favorable sites for nucleation. Some grains can accommodate more deformation than others due to their orientation (see [55]). These grains with high stored energy (highly deformed) serve as the favored locations for nucleation of new grains during static recrystallization as a result of favorable stored energy reduction through the reduction of dislocation densities.

Figures 2(a) and (b) show the microstructural representation of dislocations as a scalar quantity characterizing the work hardening of the cold rolling process. The SSD distribution seems relatively inhomogeneous as shown in figure 2(a), but agrees with the plastic strain distribution in figure 2(c). This confirms qualitatively that SSDs contribute to plastic strain in the absence of high-stress gradients [21, 56]. It has been reported that plastic flow induces the dislocation densities to be gathered along the grain boundaries [44]. Figure 2(b) shows the second type of dislocation distribution, where high-stress gradients are encountered especially near grain boundaries. Ashby [56] has shown that GNDs usually accumulate in areas of high-stress gradients to ensure strain compatibility during plastic deformation in such regions. Regions of either a denser network of dislocations (SSDs) or higher misorientation gradients (GNDs) are more likely to develop recrystallizing nuclei, which grow at the expense of regions with a low stored energy [57]. Figures 2(c) and (d) show the strain rate and stress distribution on the exterior surface of a simulation volume. It should be noted that the local variations in strain rate (figure 2(c)) and stress (figure 2(d)) display dissimilar features in the two fields [43].

3.3. Microstructural evolution

Figure 3(a) and (b) show the total dislocation distribution, \( \rho_{\text{total}}^\gamma = \rho_{\text{totad}}^\gamma + \rho_{\text{GND}}^\gamma \) the driving force for recrystallization and its correlation with the microstructure for cold rolled single-phase aluminum alloy.

Figures 3(b)–(f) show the microstructure evolution during the simulation. Modeling the nucleation presents several challenges at the level of mesoscopic simulation of microstructural evolution due to its characteristic length scale, which is on the order of 100 nm or less, smaller than the characteristic grain size after recrystallization. However, in the current
work, the nucleation of recrystallized grains is modeled by adding small subgrains to the deformed matrix at non-random positions at the beginning of the simulation (i.e. site saturated nucleation), where the SSD and GND densities are high at the beginning of the simulation. The dark regions along the grains represent regions of high stored energy (total dislocation density above $2 \times 10^{15} \text{m}^{-2}$) of the initial microstructure, figure 3(a), which is considered here to be the critical value in which recrystallization is assumed to occur. These recrystallizing subgrains are assumed to be strain free and the SSD and GND values are set to zero at each site belonging to the recrystallized subgrains. These recrystallizing nuclei can grow into the deformed material owing to the stored energy gradient, from which they are separated by high angle grain boundaries [58].

The crystallographic orientations of these subgrains are dissimilar to the deformed grains and are considered to be unchanging during the simulation. The recrystallization texture of these subgrains are chosen from a list containing typical recrystallization components in FCC materials such as Cube and R as follows: \{0°, 0°, 0/90°\}; \{0°, 22°, 0/90°\}; \{53°, 36°, 60°\} in the Bunge Euler angle convention [59, 60]. Here it should be mentioned that the ability of the nucleus to grow may also be influenced by the orientations of adjacent nuclei in the microstructure. However, the subgrains with partial high angle grain boundaries only can grow into the matrix.

Figure 2. (a) 3D statistically stored dislocation density distribution and (b) 3D geometrically necessary dislocations distribution of polycrystalline Al alloy upon cold rolling. The color bar shows the dislocation density in $\text{m}^{-2}$. (c) Von Mises stress, and (d) strain on the surface of the simulation volume.
As the simulation progresses the fraction of recrystallized grains increases from 0 to 1 as the simulation proceeds. The recrystallizing grain boundaries separate the deformed microstructure from a region that is fundamentally free of dislocations as these high angle grain boundaries move and sweep out the areas of non-zero stored energy \[57\]. Once the stored energy is consumed entirely the simulation will have a normal grain growth behavior. In this moment of the simulation, the driving force for growth is independent of the stored energy, and all the boundaries are driven with identical force \[58\]. However, the microstructure of recrystallized grains is still not fully stable, and the grain boundary energy now works as a driving force for grain growth to diminish the total area of these boundaries (decrease in the number of grains per unit volume). Hence, grain growth results in increases of the average size of recrystallized grains, creating equiaxed grains as observed in figure 3(f). The rate of growth is only controlled by the surface energy. The simulated evolved microstructure qualitatively agrees with evolved structures of AA1100 from in situ annealing as shown in figure 1. The coarsening rate of recrystallized grains is relatively slow at the late stage of simulation. This is due to the change in misorientation environment of the migrating recrystallization fronts, when the grains grow larger \[60\].

3.4. In situ microstructural evolution

For quantitative analysis of these observations two parameters are considered: the fraction of recrystallized grains and the average grain size. As can be seen in figure 4 during recrystallization as well as during the succeeding grain growth process, the average grain size of the material increases. It is commonly understood that there is an initial nucleation period, in
which the nuclei incubate, and then commence to grow at a (constant) rate overwhelming the
deformed matrix, a process that is later followed by the impingement of grains. In the present
work, the nucleation period is neglected. Nevertheless, during recrystallization for any set of
grains the average grain radius $R$ at any time $t$ can be described by [4]:

$$\langle R \rangle = G (t - t_0),$$

where $t_0$ is the nucleation time, $G$ is the rate of growth, and the grains are assumed to be
spherical. It can be seen in figure 4(a) that equation (15) is indeed fulfilled for the early
simulation regime (approximately for 120 MCS), during which recrystallization happens
(compare also to figure 5). For longer annealing times there are clear deviations. Since it is
well known that for normal grain growth the average grain radius follows a square-root law of
time, hence, the average grain area increases linearly with time, which we find indeed for longer simulation times as shown in figure 4(b).

Assuming that during the very early recrystallization regime \( n \) nuclei form in a time increment \( dt \) then the volume fraction \( f \) of transformed material is given by:

\[
 f = \frac{4}{3} \pi h G^3 \int_0^t (t - t_0)^3 dt = \frac{\pi}{3} h G^3 t^4
\]

(16a)

using the rate of growth \( G \). It should be noted that equation (16a) holds only for the early stage of recrystallization, where \( f \ll 1 \). Since we excluded this stage from the current research, we have to consider the case for higher volume fractions, where the grains may come into contact with one another and the growth slows down. Then the rate of growth is related to the fraction of untransformed material \((1 - f)\) by the Johnson–Mehl-equation, and it follows:

\[
 f = 1 - \exp \left( -\frac{\pi}{3} h G^3 t^4 \right)
\]

(16b)

This is, of course, only an approximation, where it is assumed that the grains are spherical, the nuclei are randomly distributed, the nucleation time \( t_0 \) is small, and the growth rate is constant. It does not take into account the initial condition of the material as well as the constantly changing relationship between the growing grains, the deformed matrix, and any second phases or other microstructural factors. Nevertheless, such a plot of the volume fraction of recrystallized grains versus annealing time is commonly used to characterize the progress of recrystallization. These simulated kinetics of recrystallization correspond to the phase transformation, which arises by nucleation and growth. Computationally, the recrystallization behavior is represented in a nucleation and grain growth matching display of new grains in the microstructure and continuing growth of recrystallized grains to sweep out the deformed matrix. Figure 5 shows the typical sigmoidal form of recrystallized grain fraction according to the least-squares fit of equation (16b), which characterizes the simulation results. The plot shows a 10% fraction of site saturation nuclei were assigned at time zero, followed by a rapid increase of the recrystallization rate (slope), and lastly due to impingement of growing grains (around \( t = 120 \)) a diminishing rate of recrystallization is noticed [4].

3.5. Recrystallization texture

The prediction of the texture development during recrystallization is still poor, unlike that of deformation textures. The recrystallization texture conventionally has been illustrated, but not predicted, by two competing theories of oriented growth and oriented nucleation [60–63]. The latter theory is adopted here by suggesting that favored formation of special orientations of nuclei specifies the evolved recrystallization texture [62]. Growth of nuclei into the deformed matrix leads to a drastic change in the distribution of texture within the alloy. The \( \beta \) fiber and \( \alpha \) fiber are the most significant in rolling textures for FCC metals [64]. The evolved textures are mainly responsible for the anisotropic properties (directionality) of finished products [29]. The evolved textures were measured by totaling the orientations corresponding to a recrystallized voxel.

The cube recrystallization texture is the most dominant component in metals with high stacking fault energy, such as Cu, Ni, and Al. Therefore, the manifestation of cube recrystallization is attributed to retained cube orientation of old deformed grains or recrystallization on shear bands [64]. Juul Jensen et al studied recrystallization texture development in a
severely deformed alloy, and they concluded that the recrystallized grains of the cube orientation, which were comparatively small in quantity, appeared to grow at more rapid rates than recrystallized grains of the other texture components [64]. Figure 6 shows the ODF of the evolving texture during simulation. The traditional texture components that originate during recrystallization, such as Cube and R, are clearly present. The evolved texture is determined by measuring volume fractions of recrystallized texture components. The ODF plots in the form of $\varphi_2$ sections show strong changes in texture that can occur during recrystallization of FCC metals, especially at high deformations and with a lack of alloying [2]. Figure 6 displays the ODF of a single-phase Al alloy measured after cold rolling process. The hot rolling reduction was presumed to be 70%.

The main rolling fibers of FCC metals $\alpha$ and $\beta$ are clearly visible below in figure 6 (brass, S, Cu, and Goss) along with a small fraction of the cube $\{100\} \langle 001 \rangle$ component. During cold rolling cube grains have been re-oriented to new orientations, but a number of them resisted and are still present after cold deformation (compare [29]).

4. Summary and conclusion

In the present work, two kinds of dislocation densities, namely SSDs, and GNDs, and their correlation with the structure were investigated based on the VP-FFT method. The dislocation densities were established to identify the favorable sites for nucleation. Particularly, the SSDs were used to quantify the heterogeneous distribution of the recrystallization driving force, whereas the GNDs identified orientation gradients in the microstructure due to plastic deformation.

The recrystallizing subgrains were allocated non-randomly along the grain boundaries, which was comparable to the experiments. The latter have been performed as \textit{in situ} EBSD.
experiments in order to validate the rationality of the simulation results and to clarify that recrystallization in AA1100 alloy has heterogeneous character, and depends on the SSD and GND distributions. Recrystallization arose because of growth and competition between the subgrains. Once the stored energy was consumed entirely the simulation showed a normal grain growth behavior. In this moment, the driving force for growth was found from the simulation to be independent of the stored energy, and all boundaries were driven forward with identical force.

The simulated textured was determined by weighting the recrystallized grain fractions in the structure. Even though, there are no absolute length and timescales in Potts model simulations, it is possible to conclude that the simulated behavior tends to follow the trends of the real experimental kinetics as dictated by MC time steps. The influence of nuclei orientation and growth rate of the new grains on the development of the texture during recrystallization was represented by ODFs.

The general vision of the presented quantitative modeling is to be able to optimize the microstructural features (grain size, recrystallization fraction, and crystallographic texture) during recrystallization and grain growth computationally in three dimensions in single-phase Al alloys. This simulation provides beneficial tools for understanding annealing and related phenomena in thermal treatments of rolled structures.

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