Mesosopic coupled modeling of texture formation during recrystallization considering stored energy decomposition

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Abstract

Microstructure-based simulations were performed to understand the mechanism involved with texture formation during recrystallization in polycrystalline interstitial free (IF) steel. The crystal plasticity finite element method (CPFEM) was used to simulate mesoscopic deformation with its heterogeneity. The orientation components were decomposed according to the stored deformation energy, and the results were used to define potential candidates for nucleation sites. On the basis of the oriented nucleation approach, the subsequent evolution of microstructure and texture during recrystallization was simulated with the cellular automaton (CA) method. The coupled microstructure-based simulations provided the recrystallization kinetics, grain size distribution, and crystallographic texture of the recrystallized IF steels. Those results were in good agreement with experimental results obtained from electron back scattered diffraction (EBSD). This suggests that the level of detail of the deformed state captured from the crystal plasticity FE calculation can provide enough information, in terms of local stored energy and nucleation site selection, to enable modeling of the subsequent primary recrystallization process.

Keywords: Microstructure, Recrystallization texture; Stored deformation energy; Crystal plasticity; Cellular automaton

1. Introduction

The macroscopic mechanical properties of automotive steel sheet depend strongly on microstructure and texture evolution [1,2]. To better understand their effects, the deformation and recrystallization behaviors of various metals and alloys have been widely investigated. Humphreys and Hatherly [1] reviewed recrystallization and associated annealing phenomena in the materials in their book. Hutchinson [2] provided a comprehensive review of microstructure and texture evolution in low carbon steels. In particular, it has been reported that the relative volume fractions of α -fiber texture (RD//<110>) and γ -fiber texture (ND//<111>) are critical to the drawability of interstitial free (IF) steel sheets: the γ -fiber texture improves sheet metal formability by increasing the Lankford value with little directional variation [3,4]. Duggan et al. [3-5] extensively investigated the origin of recrystallization texture in cold-rolled IF steel and reported that the grains in the γ -fiber texture exhibited larger orientation gradients than other components, and this favored the formation of nuclei which propagated into the matrix. This is the main mechanism behind the formation of dominant γ -fiber in the final recrystallization texture. Recently, an in-situ EBSD study showed that the annealing response is strongly dependent on the type and number of average orientations among the deformed γ -fiber grains in a cold-rolled Cu-added bake-hardenable steel [6].

Stored deformation energy, which is accumulated during plastic deformation, is one of the most important microstructural parameters affecting the recrystallization texture [1,7]. At the same time, the stored deformation energy in cold-rolled materials has been found to vary with crystallographic orientation [8,9]. Accordingly, a wide spectrum of experimental and computational works have been used to quantify the orientation-dependent stored deformation energy of polycrystalline materials. The orientation-dependent deformation heterogeneity can be readily characterized by EBSD analysis. In addition to computing the gradient from an orientation map, the EBSD image quality can be used as an indicator of orientation gradients, internal stresses or deformation energy

1 because indexing the Kikuchi pattern is dependent on the density of lattice defects [10-12].
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3 Following earlier work by Vatne et al. [13], Choi et al. [14,15] used a subgrain method to estimate
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5 the stored deformation energy depending on the amount of cold rolling of IF steel. The method
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7 computes the approximate dislocation density using subgrain size and mean misorientation angle,
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9 and helps to reveal the heterogeneity of intragranular deformation. However, the method is sensitive
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11 to sample contamination and the choice of subgrain identification angle.
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16 Theoretical and computational modeling is a useful alternative for quantifying the stored
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18 deformation energy. Rajmohan et al. [16] simulated texture evolution in a cold-rolled IF steel by
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20 correlating the deformation energy to the Taylor factor according to the crystal orientation. Diligent
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22 et al. [17] utilized the elasto-plastic self-consistent polycrystal model to calculate the orientation-
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24 dependent stored energy. However, such polycrystal plasticity models are unable to take into
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26 account deformation heterogeneity arising from interactions among the neighboring orientations.
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31 Meanwhile, mesoscopic microstructure-based modeling approaches such as the crystal plasticity
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33 finite element method (CPFEM), have been popular for simulating the orientation-dependent
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35 heterogeneity of deformation because one can use the crystal plasticity that naturally results in
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37 heterogeneous deformation [18]. The orientation-dependent stored energy in aluminum and IF steel
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39 was calculated using CPFEM by Sarma et al. [19] and Choi [20], respectively. Previous efforts
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41 were based on a 2-D analysis with an ideal microstructure configuration, which could not take into
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43 account the interaction between a grain and all of its surrounding grains, i.e., its neighborhood.
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48 The mesoscopic simulation of recrystallization and grain growth was advanced by the pioneering
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50 work of Anderson et al. [21] who first applied the Monte Carlo (or Potts) model to problems of
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52 grain growth and then primary recrystallization [22]. Rollett et al. [23,24] presented an extensive
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54 overview of mesoscopic simulation for recrystallization. They also proposed a hybrid of the Monte
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56 Carlo and cellular automaton (CA) models to improve the simulation of the mesoscopic behavior of
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1 recrystallization and grain growth, considering both curvature-driven and stored energy-driven
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3 grain boundary migration. Raabe and Becker [25] published a method that coupled CPFEM and CA
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5 for simulating primary recrystallization after deformation in an aluminum alloy. Holm et al. [26]
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7 and then Takaki and Tomita [27] simulated abnormal subgrain growth to study the nucleation
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9 process in a face-centered cubic (fcc) metal, based on coupled simulations with phase-field and
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11 CPFEM. Takaki and Tomita only focused on simulating recrystallization kinetics, without in-depth
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13 discussion about the recrystallization texture or experimental observation. In a follow-up to the
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15 earlier paper, Wang et al. [28] showed how the statistics of abnormal subgrain growth could be
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17 combined with information on subgrain size and misorientation to predict grain sizes in primary
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19 recrystallization. Recently, Permann et al. [29] developed a re-mapping algorithm for the phase
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21 field model using FEM to simulate grain growth. Scholtes et al. [30] reported a fully 3-D modelling
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23 of static recrystallization considering stored energy fields.
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30 In this study, we present (i) experimental observations of the recrystallization behavior in IF steel
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32 that was cold-rolled to true strain levels of 0.7 and 1.6, and subjected to annealing at 700 °C and
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34 800 °C, using EBSD analysis; and (ii) a 3-D microstructure-based integrated modeling approach to
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36 simulate the deformed substructure, stored deformation energy, and microstructure evolution. Most
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38 importantly, the coupling of theoretical modeling and experimental observation helps to elucidate
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40 the texture evolution during primary recrystallization.
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2. Experimental methods

2.1 Sample preparation

The material for the experiments was as-received IF steel with an average grain size of around 30 μm , produced on a hot rolling line at the POSCO steel company. Its chemical composition is given in Table 1. The material was further deformed by cold rolling to low and high true strains of $\varepsilon = 0.7$ and $\varepsilon = 1.6$, corresponding to reductions in thickness of 50 % and 80 %, respectively. Since the amount of cold rolling deformation is an important factor in the recrystallization behavior, we selected a reduction of 80 % in plate thickness, which corresponds to a true strain level of $\varepsilon = 1.6$. This was found to optimize the volume fraction of the γ -fiber and accordingly the drawability of the sample [3]. All the samples were fully annealed for 1 h at a temperature above 700 $^{\circ}\text{C}$, and small samples cut from the cold-rolled sheet were isothermally annealed at 700 $^{\circ}\text{C}$ and 800 $^{\circ}\text{C}$ for various times to observe the evolution in microstructure during primary recrystallization.

2.2 EBSD analyses

All the samples were sectioned and examined on the plane perpendicular to the transverse direction (TD) as shown in Fig. 1(a). The microstructure measurements were made with an EBSD system (EDAX-TSL/Hikari) attached to a field emission scanning electron microscope (FESEM, FEI/Nova 230). For the smaller strain ($\varepsilon = 0.7$), EBSD maps of two neighboring scan areas of 210 $\mu\text{m} \times 410 \mu\text{m}$ were measured, with step sizes of 0.4 μm in the deformed sample, and 1 to 2 μm for the rest. Then, the neighboring areas were merged to obtain a total scan area of 380 $\mu\text{m} \times 400 \mu\text{m}$ to improve the accuracy of the measurement. Note that 400~2,300 grains were included in each measurement. For the higher strain ($\varepsilon = 1.6$), the EBSD maps were measured with a scan area of 200 $\mu\text{m} \times 400 \mu\text{m}$, and with step sizes of 0.4 μm in the sample in which the recrystallized fraction was below 30%, and 1 μm for the rest, consisting of 900-5,000 grains.

Before the analyses of the EBSD data, a cleanup procedure consisting of grain confidence index standardization, followed by neighbor orientation correlation, was applied with a grain misorientation of 5°, an equivalent grain size of minimum 4 pixels, and a minimum confidence index of 0.1. In this procedure, the orientations of isolated pixels around identified grains were changed to match that of adjacent neighbors. A fine step size was used to ensure successful orientation correlation during the cleanup procedure. The analyses of the EBSD data were conducted using EDAX TSL OIM Analysis v.6.1. A more detailed description of the experimental procedure and EBSD data analysis can be found in [31].

3. Microstructure-based models

3.1 Crystal plasticity finite element model (CPFEM)

Crystal plasticity theory is well established, and details can be found in the literature [32-36]. In the present study, the crystal plasticity formulation described in reference [37-39] was incorporated into an in-house FE code, CAMPform3D [40] in order to define the constitutive response at each integration point having an individual crystallographic orientation. It should be mentioned that remeshing was indispensable for simulating large deformation up to $\varepsilon = 1.6$. When the reduction in thickness reached 50 %, remeshing was applied and the state variables were transferred to the new mesh by the previously proposed direct data mapping method [39].

In the constitutive model of rate-dependent materials, to describe the shearing kinetics on the active slip systems, the dependence of the slip rate on the resolved shear stress and the resistance to shearing is given in the form of a power law [34] as follows:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \frac{\tau^{\alpha}}{\tau_R^{\alpha}} \left| \frac{\tau^{\alpha}}{\tau_R^{\alpha}} \right|^{\frac{1}{m}-1} \quad (1)$$

where $\dot{\gamma}_0^\alpha$ is the reference shear rate for the plastic slip, τ^α is the resolved shear stress, τ_R^α is the reference shear stress on the α -th slip system, and m is the rate sensitivity parameter.

Self and latent hardening characteristics of the material are considered in terms of the evolution of the resistance to shearing, as suggested by Peirce et al. [36]:

$$\dot{\tau}_R^\alpha = \sum_{\beta=1}^n \mathbf{h}_{\alpha\beta} \dot{\gamma}^\beta \quad (2)$$

where $\mathbf{h}_{\alpha\beta}$ is the hardening matrix including the interactions among the slip systems.

$$\mathbf{h}_{\alpha\beta} = qh + (1-q)h\delta_{\alpha\beta} \quad (3)$$

where $\delta_{\alpha\beta}$ is the Kronecker delta, h is the hardening modulus, and q is the latent hardening rate due to the slip activity on other slip systems. Here, a q value of 1.4 was used for texture analyses of the polycrystals [36,41]. The hardening law proposed by Voce [42] was adopted in this study.

$$h = h_0 \left(1 - \frac{\tau_R^\alpha}{\tau_s} \right)^a \quad (4)$$

where h_0 is the initial hardening rate, τ_s is the saturation value of the current strain hardened state of the slip system, and a is the hardening exponent. Note that the crystallographic slip was restricted to the 12 $\{110\} \langle 111 \rangle$ and 12 $\{112\} \langle 111 \rangle$ slip systems. The material parameters used in the CPFE analysis are given in Table 2 [43].

The stored deformation energy resulting from the plastic deformation was estimated using the average resolved shear stress $\bar{\tau}$ which is proportional to the square root of the dislocation density, as follows [1]:

$$\bar{\tau} = \frac{1}{n} \sum_{\alpha=1}^n \tau_R^\alpha = \frac{1}{2} \mu b \sqrt{\rho} \quad (5)$$

where μ is the shear modulus; b is the Burgers vector; ρ is the dislocation density. Based on the standard approximation for the dislocation energy per unit length, the stored deformation energy

E_D is given by $E_D = 0.5\mu b^2 \rho$. In combination with Eq. (5), the stored deformation energy is as follows:

$$E_D = \frac{2\bar{\epsilon}^2}{\mu} \quad (6)$$

The mesoscopic deformation heterogeneity over the microstructure can be expressed in terms of the stored deformation energy and orientation distributions over the representative volume element (RVE). Note that the deformed states at each integration point, as calculated with CPFEM, were provided as the initial microstructure in the CA simulation described in section 3.2.

3.2 Cellular automaton (CA)

Starting from the deformed state described by the distributions of orientation, and the stored deformation energy calculated by CPFEM, the microstructure and texture evolution during primary recrystallization was simulated using probabilistic CA with the Moore neighbor rule. The nucleation was assumed to take place in a continuous and probabilistic fashion. The normalized parameter P_N at each site was calculated as follows:

$$P_N = \frac{E_D - E_D^{\min}}{E_D^{\max} - E_D^{\min}} \quad (7)$$

where E_D is the stored deformation energy at the site, $E_D^{\min}$ and $E_D^{\max}$ are the minimum and maximum stored deformation energies, respectively. Among the sites where the accumulated deformation energy was higher than a critical value, E_D^c , a certain number of cells for each time increment were chosen to be nuclei when the normalized parameter was higher than a randomly generated number between 0 and 1. Note that requiring a minimum level of stored energy is equivalent to requiring a minimum amount of strain to be accumulated before recrystallization can initiate. This is reasonable in that orientation gradients increase with strain and nearly linearly at

small strains [44]. The nucleation of new grains in recrystallization is necessarily heterogeneous [7] because of the requirement for a mobile high angle boundary around the nucleus, as well as sufficient stored energy to allow the boundary to move. Thus stored energy appears both directly as a driving force and indirectly via the need for a mobile high angle boundary around each new grain.

For the cells that satisfied the nucleation criterion, the state of the cell was switched to be recrystallized without any change in orientation, dropping the stored deformation energy to zero. The rate of nucleation is given by using the following phenomenological relationship [45]:

$$\dot{N} = C_0 (E_D - E_D^C) \exp\left(-\frac{Q_{RX}^N}{RT}\right) \quad (8)$$

where C_0 is the nucleation rate constant, E_D is the stored deformation energy, E_D^C is the critical stored energy, Q_{RX}^N is the activation energy for nucleation, R is the universal gas constant, and T is the temperature.

The rate of grain boundary migration v is proportional to the driving force p with the grain boundary mobility m ($v = mp$). The driving force for primary recrystallization is predominantly stored deformation energy in the form of dislocation density, which is the same as E_D given in Eq. 6. The grain boundary mobility is a function of the disorientation $\Delta\theta$ between each grain boundary site and its neighboring cells and T , as follows [46]:

$$m = m_0 \exp\left(-\frac{Q_b}{kT}\right) \left[1 - \exp\left\{5\left(\frac{\Delta\theta}{15}\right)^4\right\}\right] \quad (9)$$

where m_0 is the constant for high angle boundary; Q_b is the activation energy for grain boundary movement; k is Boltzmann's constant. To calculate disorientation, the Euler angles were converted into the orientation matrix and then the misorientation matrix M_{12} was computed from the neighboring orientations of site 1 and site 2, as follows:

$$M_{12} = g_2 g_1^{-1} \quad (10)$$

where g_1 and g_2 are the orientation matrices for each site. The rotation angle $\Delta\theta$ was extracted from the misorientation matrix M_{12} in the standard manner as follows:

$$\Delta\theta = \arccos\{(tr(M_{12})-1)/2\} \quad (11)$$

The minimum among all the possible 24 crystallographically equivalent misorientations was selected, taking cubic crystal symmetry into account. Values for the various parameters in the CA model are given in Table 3 [47,48].

3.3 Simulation procedure

The microstructure and texture of the as-received IF steel measured by EBSD and XRD are shown in Fig. 1(a)-(b). The initial microstructure was found to be an almost random orientation distribution with an equiaxed grain morphology. The RVE for the initial microstructure was generated by a Voronoi tessellation [49]. The FE mesh of the RVE was made up of 8,000 eight-node 3-D solid cuboidal elements, whose the number of integration points was eight for full integration, as shown in Fig. 1(c). The initial dimension of each RVE was $200 \times 200 \times 400 \mu\text{m}^3$ in a cuboidal shape, comprised of 1,200 grains with an average grain size of about $30 \mu\text{m}$. The RVE was assumed to have a random orientation distribution since the one measured for the as-received IF steel was almost random, as shown in Fig. 1(b).

Three dimensional analysis of the channel die compression of the RVE was carried out with CPFEM. The interior nodes on the planes normal to the normal direction (ND) at $z = 400 \mu\text{m}$ were allowed to move in the ND. The interior nodes on the planes normal to the rolling direction (RD) at $x = 200 \mu\text{m}$ were constrained to exist on a plane normal to the RD. The interior nodes on the planes normal to the transverse direction (TD) at $y = 0$ and $y = 200 \mu\text{m}$ were constrained in the TD while the lateral displacements on the planes were allowed to move freely. The RVE was deformed to

1 reduce the initial thickness by 50% and 80%, corresponding to compressive true strains of $\varepsilon = 0.7$
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3 and $\varepsilon = 1.6$, respectively.
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6 The deformed states at each integration point, as calculated with CPFEM, was provided as the
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8 initial microstructure in the CA simulation. The state variables calculated from the CPFEM analysis,
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10 i.e., the Euler angles and stored deformation energy, were transferred onto the nearest CA lattice
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12 cell. When mapping a continuous description on a discrete grid, the cell size of the CA grid was
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14 more refined compared to the size of the finite element. The physical length of each cell was 1.07
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16 μm while the size of the finite element was 2.69 μm . The CA simulations were conducted on grids
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18 with dimensions of 200 x 100 x 100 and 500 x 100 x 40 for $\varepsilon = 0.7$ and $\varepsilon = 1.6$, respectively. The
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20 annealing was assumed to be isothermal.
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27 **4. Results**

28 *4.1 Measurement of microstructure, grain size, kinetics, and texture*

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33 Figures 2 and 3 show the microstructure evolution during annealing at 700 °C for the specimens
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35 strained to $\varepsilon = 0.7$ and $\varepsilon = 1.6$, respectively. In each figure the upper row displays inverse pole
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37 figures (IPF) relative to the ND and the lower row displays the pattern quality (PQ) with grain
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39 boundaries. The cold-rolled microstructure of the single-phase polycrystalline IF steel exhibited
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41 well-defined substructures, in which high angle grain and dislocation boundaries were aligned along
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43 with the RD. It may have a high degree of stored deformation energy, as pointed out by Hurley and
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45 Humphreys [50].
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50 The cold-rolled microstructure consists of two apparently different regions. As shown in Fig.
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52 4(a), for the specimen strained to $\varepsilon = 1.6$, the cold rolling texture contains a strong α -fiber (~48 %)
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54 and a relatively weak γ -fiber (~29 %); the corresponding regions are colored in yellow and green,
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56 respectively. The distributions of kernel average misorientation (KAM) in Fig. 4(b)-(c) indicate a
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large amount of orientation spread and subdivision into subgrains, found mainly in the γ -fiber regions. This is quantitatively evaluated in Fig. 4(d), in which the KAM value is plotted in orientation space ($\varphi_2 = 45^\circ$ ODF section) for orientations with an intensity above 1.0 MRD.

As shown in Fig. 4(e), the average values of KAM were found to be approximately 2.3° and 2.9° for the α -fiber and γ -fiber regions, respectively, showing that larger orientation gradients exist in the gamma fiber, as was noted by Duggan *et al.* [3]. Here, KAM is the average misorientation between a material point and all orientations within the third nearest neighbors, excluding values greater than 5° .

The recrystallization kinetics were determined from Vickers microhardness measurements and the adaptive identification of deformed and recrystallized grains using the intragranular orientation spread, with the criterion that grain orientation spread (GOS) is below a critical value for the recrystallized grains. GOS is defined as the average misorientation between the average orientation of a grain and the orientation of each individual measurement point within the grain. A critical value of $\text{GOS} = 2.5^\circ$ was found to provide a good identification of the recrystallized grains according to [31].

In the early stage of annealing, nucleation took place predominantly in the γ -fiber region and the nuclei propagated into the deformed matrix. Interestingly, the recrystallizing grains showed an elliptical morphology with the major axis aligned with the RD. For the highly strained sample ($\varepsilon = 1.6$), the anisotropic grain morphology was more pronounced and a strong texture was observed at the end of recrystallization.

Figure 5 shows the texture development in the samples strained to $\varepsilon = 0.7$ and $\varepsilon = 1.6$ by cold rolling and full annealing at 700°C and 800°C in terms of the $\varphi_2 = 45^\circ$ section of the orientation distribution function (ODF). The deformation textures of the cold-rolled samples mainly consist of α -fiber with a reinforcement of the $\{001\}\langle 110 \rangle$ component and γ -fiber, whereas the

recrystallization texture reveal the definite disappearance of the α -fiber texture and a strengthening of the γ -fiber. For the high strain sample ($\varepsilon = 1.6$), the texture had two times higher intensity compared to the low strain case ($\varepsilon = 0.7$). Regardless of the annealing temperature, the recrystallization textures showed almost the same pattern of contours. Thus, the influence of the annealing temperature on the grain size and recrystallization texture was negligible for the present material, which is consistent with previous studies [3].

Figure 6 shows the progressive texture evolution with respect to the recrystallized fraction. The texture components of the deformed and recrystallized grains were discriminated using a method previously developed by the authors [31]. For the recrystallized grains only, most of the orientations at the incipient stage ($X_v = 20\%$) belong to the γ -fiber with reinforcement of the $\{111\} \langle 112 \rangle$ component, and are similar to the final recrystallization texture. It is evident that the texture of the nuclei is similar to the final recrystallization texture, which supports the oriented nucleation theory [1]. Meanwhile, in the case of the deformed grains only, most of the orientations belong to the α -fiber texture with a reinforcement of the $\{001\} \langle 110 \rangle$ component, which remains non-recrystallized even at the final stage ($X_v = 97\%$). Thus, this clearly shows that the nucleation takes place predominantly in the γ -fiber texture components, and results in the strong development of the γ -fiber texture.

4.2 Simulation of deformation heterogeneity and recrystallization texture

Figure 7 shows microstructure changes in terms of the RVE in RD and ND IPF maps during channel die compression. Although the RVE is subjected to channel die compression from the macroscopic point of view, strain localization and out-of-plane shear deformation are evident owing to the orientation-dependent anisotropy, needed to maintain compatibility and equilibrium

1 throughout the microstructure. As the reduction in thickness increases, both α -fiber and γ -fiber
2 textures are developed, as shown in Fig. 7.
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6 Figure 8 shows the simulated deformation heterogeneity in terms of the lattice rotation
7 magnitude. Here, lattice rotation magnitude means the minimum rotation angle associated with the
8 disorientation between orientations for a material point before and after deformation. This
9 represents the magnitude of the lattice reorientation that occurs as a result of slip. The rotation angle
10 was calculated with Eqs. 10-11. The heavily heterogeneous distribution of the lattice rotation
11 implies severely localized straining [15,20]. The lattice rotation map reveals in-grain orientation
12 gradients and the inhomogeneous nature of deformation, which depends on the initial orientation.
13 Thus, it suggests that stored deformation energy is accumulated in a heterogeneous manner, as is
14 evident from experiments [51,52].
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28 Figure 9 shows the simulated stored deformation energy in the RVE and the corresponding
29 histogram, which represents the volume fraction as a function of the stored deformation energy.
30 Note that the stored deformation energy, which is related to the dislocation density caused by the
31 plastic deformation, was calculated with Eqs. 5-6. The results show that the distribution of stored
32 deformation energy was inhomogeneous at all strain levels. This is likely because of the combined
33 dependence of total slip on the grain orientation, and the influence of neighboring grains on each
34 individual grain. The histogram in Fig. 9(d) shows that the distribution of stored deformation
35 energy is approximately normal, with mean values of 0.95, 1.68 and 2.23 MJ/m³ for the strain levels
36 of $\varepsilon = 0.1$, $\varepsilon = 0.7$ and $\varepsilon = 1.6$, respectively.
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52 **5. Discussion**

53 *5.1 Influence of grain orientation on stored deformation energy*

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First we discuss the dependence of the stored deformation energy on the crystallographic orientation. Figure 10 shows the variations in texture depending on the level of stored deformation energy, divided into four classes of cumulative frequency, i.e., 5 %, 10 %, 90 %, and 95 %. Note that the texture components were partitioned from the overall texture at $\varepsilon = 1.6$, as shown in Fig. 10(a). The overall simulated deformation texture, seen in Fig. 10(a), contains a strong α -fiber texture and a relatively weak γ -fiber texture. This is in good agreement with the XRD and EBSD experimental observations in Figs. 5 and 6. It is clear that the deformation texture significantly depends on the stored energy. The texture changes significantly from the α -fiber to the γ -fiber texture as the stored energy increases from 5 to 95% of the range, as shown in Fig. 10(b)-(e).

Figure 11 shows the contours of the average stored energy per point in orientation space ($\varphi_2 = 45^\circ$ ODF section) where the intensity is above 1.0 MRD. This clearly reveals that the γ -fiber orientations have significantly higher stored energy than the α -fiber orientations. This helps to explain why the nucleation density is higher in the γ -fiber than in the α -fiber. Nevertheless it is also relevant that orientation gradients are stronger in the γ -fiber because of its propensity for shear banding [3], which also promotes nucleation; this is assumed to be effectively included in our model via the nucleation criterion in Eqs. 7 and 8.

5.2 Recrystallization kinetics, grain size, and texture

Figure 12 shows simulated microstructure evolution during the primary recrystallization of the RVEs initially strained to $\varepsilon = 0.7$ and $\varepsilon = 1.6$. The non-random spatial distribution of nuclei generated as a consequence of their sensitivity to stored energy, and the anisotropic migration of the boundary of recrystallizing grains, as observed in the experimental data, are shown in Figs. 2-3. In particular, it can be seen that the level of heterogeneity and anisotropy are more pronounced for the RVE strained to $\varepsilon = 1.6$. The majority of the nuclei clusters which formed early in recrystallization

1 coalesced into large recrystallizing grains. Thus, owing to the inhomogeneous distribution of stored
2 deformation energy, the recrystallizing grains had varying velocities along their perimeters and
3 hence their propagation into the deformed regions varied from location to location with variations
4 in mobility and stored energy.
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10 Figure 13 compares the recrystallization kinetics from the experiments and the simulations as a
11 function of annealing time. The sigmoidal curves correspond to an initially increasing rate of
12 recrystallization, with an inflection into a linear region, and finally a decreasing rate of
13 recrystallization. This is consistent with the recrystallization kinetics being controlled by nucleation
14 and growth in the classical manner. Clearly the rates vary with time and location in a discontinuous
15 and inhomogeneous fashion. Good agreement between the simulations and the experiments is
16 apparent despite the complex phenomena involved.
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27 Figure 14 shows a comparison between experiment and simulation of the grain size distribution
28 after full annealing at 700 °C. It shows that the grain size is smaller and more uniformly distributed
29 for the case of high strain ($\epsilon = 1.6$) compared to that of the low strain ($\epsilon = 0.7$). This is likely due to
30 the higher nucleation density at the higher strain. It is notable that the simulated grain size
31 distribution, as well as the average grain size, is well matched to the experimental results.
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40 Figure 15 shows the strong γ -fiber textures in the recrystallized IF steel. Both the simulated and
41 the measured ones are in good qualitative agreement, which supports the mesoscopic mechanism
42 for the formation of the recrystallization texture, as discussed earlier, based on the measured ODFs,
43 in Figs. 5 and 6. Accordingly, these simulations demonstrate that the final recrystallization texture
44 can be explained by the preferential nucleation of recrystallization in the γ -fiber texture components
45 which have high stored energy.
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54 It should be mentioned that the simulation quantitatively overestimates the intensity of the γ -
55 fiber, i.e., $(111)[1\bar{1}0]$ and $(111)[\bar{1}\bar{1}2]$. Such discrepancies can be caused by (i) overestimating the
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1 stored deformation energy of the γ -fiber texture components, and (ii) limited consideration of the
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3 shear band and grain partitioning associated with inhomogeneous deformation at the high
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5 deformation level. Nucleation can occur in regions with various orientation components, including
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7 the γ -fiber textures. Indeed, the potential sites for nucleation are known to be biased towards the
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9 vicinity of grain boundaries, large particles, and the edges of shear bands [1,5]. In future versions of
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11 this modeling approach, we will explore adding a criterion for nucleation that is sensitive to
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13 orientation gradients in the microstructure. There is also the possibility that numerical factors
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15 contribute to the discrepancy, such as low resolution when representing the RVE and errors
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17 involved with remeshing and data mapping.
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25 **6. Conclusions**

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27 The microstructure and texture evolution that occurs during primary recrystallization of an IF
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29 steel was investigated using both experiments and microstructure-based modeling. The
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31 experimental data were obtained for specimens cold-rolled to the true strains of 0.7 and 1.6 and
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33 annealed at 700 °C and 800 °C. The main conclusions of this study are as follows:
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37 1) The annealing temperature mainly affects the recrystallization kinetics, but has a negligible
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39 effect on the grain size or recrystallization texture. This reinforces the understanding that
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41 recrystallization as a process is controlled by the microstructure inherited from the prior
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43 deformation.
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47 2) The CPFEM simulations showed that the stored energy varied appreciably depending on the
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49 texture components. The highest stored energy was found in the γ -fiber, which corresponded with
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51 the highest nucleation densities, as observed experimentally.
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55 3) The subsequent microstructure and texture evolution during primary recrystallization was
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57 simulated by CA. The simulation showed fairly good agreement with the experimental results in
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terms of kinetics, grain size distribution, and orientation distribution albeit with an overestimated texture intensity.

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Table 1 Chemical composition of IF steel used in the present study.

Elements	C	Mn	P	S	Si	Al	Ti	N
wt %	0.0023	0.079	0.0118	0.0061	0.005	0.026	0.021	0.1115

Table 2 Parameters in the hardening model for CPFEE analysis [32].

Rate sensitivity (m)	Reference shear rate ($\dot{\gamma}_0, s^{-1}$)	Initial shear stress (τ_0, MPa)	Saturated shear stress (τ_s, MPa)	Initial hardening rate (h_0, MPa)	Hardening exponent (a)
0.05	0.001	18	81	141	0.1

Table 3 Parameters used for CA analysis [47,48].

Shear modulus (μ, Nm^{-2})	Burgers vector (b, m)	Constant for high angle grain boundary ($m_0, m^3s^{-1}N^{-1}$)	Nucleation rate constant ($C_0, J^{-1}s^{-1}$)	Critical stored energy (E_D^C, Jm^{-3})	Activation energy for nucleation (Q_{RX}^N, J)	Activation energy of grain boundary movement (Q_b, J)
3.2×10^{10}	2.58×10^{-10}	9.0×10^{-8}	6.1×10^{13}	1.67×10^6	2.33×10^{-19}	1.99×10^{-19}

Figure Captions

Fig. 1 The initial microstructure and texture of as-received IF steel sheet measured by (a) EBSD and (b) XRD, respectively and (c) the representative volume element (RVE) comprised of 1200 grains used in the CPFE simulation.

Fig. 2 Microstructure evolution (upper: inverse pole figure, IPF; lower: pattern quality, PQ) at 700 °C, $\varepsilon = 0.7$ after: (a) 0, (b) 300, (c) 600, (d) 120, and (e) 3600 sec. X_v is the recrystallized fraction.

Fig. 3 Microstructure evolution at 700 °C (upper: inverse pole figure, IPF; lower: pattern quality, PQ), $\varepsilon = 1.6$ after: (a) 0, (b) 110, (c) 180, (d) 210, and (e) 600 sec. (X_v : recrystallized fraction).

Fig. 4 Cold-rolled microstructure for $\varepsilon = 1.6$: (a) orientations close to the α -fiber (yellow) and to the γ -fiber (green) with a maximum deviation of 15°, (b) spatial distribution of KAM for α -fiber, (c) spatial distribution of KAM for γ -fiber, (d) contours of the KAM per point in orientation space ($\varphi_2 = 45^\circ$ ODF section) for orientations with intensity above 1.0 MRD, and (e) frequency distributions of KAM.

Fig. 5 Texture development (XRD measurements) after the cold rolling and full annealing at 700 °C and 800 °C plotted in the $\varphi_2 = 45^\circ$ ODF section.

Fig. 6 Texture evolution at 700 °C ($\varepsilon = 1.6$) plotted in the $\varphi_2 = 45^\circ$ ODF section. (X_v recrystallized fraction).

Fig. 7 Simulations of microstructure evolution during channel die compression in terms of RD (upper) and ND (lower) IPF maps at reductions in thickness of (a) $\varepsilon = 0.1$, (b) $\varepsilon = 0.4$, (c) $\varepsilon = 0.7$, and (d) $\varepsilon = 1.6$.

Fig. 8 Simulated deformation heterogeneity in terms of rotation angle map of the RVE strained to (a) $\varepsilon = 0.1$, (b) $\varepsilon = 0.35$, (d) $\varepsilon = 0.7$, and (d) $\varepsilon = 1.6$.

Fig. 9 Simulated distribution of the stored deformation energy of the RVE strained to (a) $\varepsilon = 0.1$, (b) $\varepsilon = 0.7$, (c) $\varepsilon = 1.6$, and (d) the corresponding histogram.

Fig. 10 Partitioning of the simulated texture components in $\varphi_2 = 45^\circ$ ODF section according to the stored energy level: (a) all energy levels, (b) below 5 %, (c) below 10 %, (d) above 90 %, and (e) above 95 %. ($\varepsilon = 1.6$). The highest energy levels are found exclusively in the gamma fiber.

Fig. 11 Contours of the average stored energy per point in orientation space ($\varphi_2 = 45^\circ$ ODF section) where intensity is above 1.0 MRD.

Fig. 12 Simulated microstructure evolution during the primary recrystallization of the microstructures initially strained to (a) $\varepsilon = 0.7$ and (b) $\varepsilon = 1.6$.

Fig. 13 Comparison between experimental and simulated recrystallization kinetics of the microstructures initially strained to (a) $\varepsilon = 0.7$ and (b) $\varepsilon = 1.6$.

Fig. 14 Comparison between experimental and simulated grain size distributions of fully recrystallized microstructures initially strained to (a) $\varepsilon = 0.7$ and (b) $\varepsilon = 1.6$.

Fig. 15 Comparison between experimental and simulated texture developments of fully recrystallized microstructures initially strained to (a) $\varepsilon = 0.7$ and (b) $\varepsilon = 1.6$.

Figure

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5

(a) $X_v=0\%$ (b) $X_v=20\%$ (c) $X_v=51\%$ (d) $X_v=69\%$ (e) $X_v=97\%$

I. Both deformed and recrystallized grains

Levels:

- 12.000
- 10.000
- 8.000
- 6.000
- 4.000
- 2.000
- 1.000

II. Recrystallized grains only

III. Deformed grains only

Fig. 6

Fig. 7

Fig. 8

Fig. 9

Fig. 10

Fig. 11

Fig. 12

Fig. 13

Fig. 14

Fig. 15

*Graphical Abstracts

CPFEM (crystal plasticity finite element method) simulation

CA (Cellular automata) simulation