Multi-Phase-Field Simulation of Flow Stress and Microstructural Evolution during Deformation-Induced Ferrite Transformation in a Fe–C Alloy

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Deformation-induced ferrite transformation (DIFT) is one of the most effective ways of refining ferrite grains in steel. In this study, we employed a multi-phase-field (MPF) model to simulate both variations in macroscopic flow stress and microstructural evolution during DIFT. Using the MPF model, two-dimensional simulations of DIFT in a Fe–C alloy were performed to investigate the effects of strain rate, austenite grain size, and dynamic recrystallization (DRX) of the ferrite phase on flow stress curve and ferrite grain size. The results demonstrated that increasing the rate of ferrite nucleation by increasing the strain rate and reducing the austenite grain size is essential to obtaining fine-grained ferrite. The results of the simulations also indicated that it is important to reduce the interfacial mobility and increase the nucleation rate of the ferrite grains subjected to DRX in order to obtain ultrafine-grained ferrite by DIFT when it is accompanied by DRX of the ferrite phase. Thus, the MPF model is an effective tool for elucidating the correlation between the variation in the flow stress and the evolution of the ferrite grains during DIFT.

KEY WORDS: multi-phase-field method; deformation-induced ferrite transformation; dynamic recrystallization; ultrafine-grained ferrite; flow stress curve.

1. Introduction

The mechanical properties of steel are strongly affected by distribution and morphology of its microstructure. In particular, the grain size of the ferrite phase of steel has a significant effect on its strength. Several techniques for grain refinement have been investigated intensively, as the refinement of the ferrite grains is one of the most effective ways of increasing steel strength. Although a number of methods have been proposed for producing ultrafine-grained ferrite, the deformation-induced ferrite transformation (DIFT) of the austenite phase has attracted a lot of attention.1–5) The DIFT is known to be a highly effective way of obtaining fine-grained ferrite with an average grain size of less than 5 μm.5–8) However, because plastic deformation and the phase transformation occur simultaneously during the DIFT, the kinetics of the DIFT are influenced by a number of factors such as the temperature, the strain rate, and the austenite grain size (AGS). Moreover, it has been reported that, in the case of plain low-carbon steels, the dynamic recrystallization (DRX) of the austenite and ferrite phases also occurs during the DIFT. The DIFT and DRX also influence dynamic softening.9) Therefore, it is very difficult to study the behaviors of these phenomena experimentally.

Consequently, the DIFT has been studied using numerical modeling and simulations. In a previous study on the numerical modeling of the DIFT, Tong et al. developed a Monte Carlo (MC) model of the DIFT.10) They investigated the effects of the strain rate, the nucleation rate of the ferrite grains, dynamic recovery, and the DRX of the austenite phase on the kinetics of the DIFT. Recently, Zheng et al. proposed a cellular automaton (CA) model and used it to simulate the DIFT as well as the DRX of the ferrite phase.11,12) However, it has been pointed out that using CA and MC models leads to problems when modeling, on the absolute time scale, the curvature-driven growth of the grain boundaries.13) These problems are serious shortcomings when it comes to quantitatively simulating the shrinking and coarsening of the ferrite grains formed by the DIFT and DRX. Furthermore, even though the flow stress behavior is a good indicator of the DIFT,9) the correlation between the variation in the flow stress and the DIFT behavior has not been analyzed sufficiently yet.

The multi-phase-field (MPF) model, on the other hand, has recently been recognized as being very effective when modeling the microstructural evolution that occurs during solidification and phase transformation in various materials.14,15) Using the MPF method, the migration of the grain boundaries owing to the curvature of the interface can be simulated in real time. A few MPF models describing the microstructural evolution during plastic deformation have

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been developed recently. Takaki et al. proposed a MPF-DRX model, which reproduces grain growth and the evolution of flow stress during DRX.\textsuperscript{16–19} Further, Busso et al. developed a sophisticated model of DRX by coupling the MPF method with a crystal plasticity finite element method.\textsuperscript{20,21} However, to the best of our knowledge, no study has used a MPF model to simulate the DIFT.

Recently, we have proposed a MPF model to simulate the microstructural evolution that occurs during the DIFT as well as the macroscopic flow stress on the basis of the MPF-DRX model proposed by Takaki et al.\textsuperscript{16,22} In this paper, a two-dimensional MPF-based simulation of the DIFT was performed using the proposed model in order to clarify the effects of deformation and microstructural parameters on the DIFT behavior. The results of the simulations proved that the proposed MPF model could elucidate the effects of the strain rate, the AGS, and the DRX of the ferrite phase on the evolution of the microstructure and the variation in the flow stress during the DIFT.

2. Material and Methods

2.1. Multi-Phase-Field Modeling of Ferrite Grain Growth

Once a ferrite grain is nucleated by the static austenite-to-ferrite transformation, the DIFT, and DRX, the grain grows into the austenite phase. During the growth of the ferrite grain, carbon atoms diffuse from the ferrite phase into the austenite phase. This type of grain growth and carbon diffusion were simulated using the MPF method. To simulate the growth of the ferrite grain, the generalized MPF model proposed by Steinbach et al.\textsuperscript{23} was used. In this MPF model, the total free energy of the system, \( G \), is defined by the Ginzburg-Landau free energy functional, which is given by the sum of the gradient energy, the potential energy, and the bulk free energy as follows:

\[
G = \int_V \left( \sum_{i=1}^{N} \sum_{k=1}^{N} \left( \frac{-a_j^2}{2} \nabla \phi_i \cdot \nabla \phi_k \right) + \sum_{i=1}^{N} \left( W_{ij} \phi_i \phi_k + g_{bulk} \right) \right) dV
\]

Here, we use \( N \) phase-field variables, \( \phi_i \) (\( i = 1, 2, 3, \ldots, N \)), \( \phi_i \) describes a fraction of the \( i \)th crystal grain. The phase-field variables vary smoothly across an interface, from \( \phi_i = 1 \) in the \( i \)th grain to \( \phi_i = 0 \) in the other grains. All the phase-field variables have to satisfy the following constraint at all computational grids:

\[
\sum_{i=1}^{N} \phi_i = 1
\]

Here, \( a_j \) and \( W_{ij} \) are the gradient energy coefficient and the potential height, respectively. These parameters are related to the interfacial energy, \( \sigma_{ij} \), and the interfacial thickness, \( \delta \), as follows:

\[
a_j = \frac{\pi}{2} \sqrt{2\delta\sigma_{ij}}
\]

\[
W_{ij} = \frac{4\sigma_{ij}}{\delta}
\]

Assuming that the microstructural evolution proceeds so that the total free energy decreases monotonically with time, the time-evolution equation for the phase-field variable can be written as

\[
\frac{\partial \phi_i}{\partial t} = -\sum_{j=1}^{N} \frac{M_{ij}^s}{n} \frac{\partial E_{chem}}{\partial \phi_j} + \sum_{j=1}^{N} M_{ij} \frac{\partial E_{store}}{\partial \phi_j} + \sum_{j=1}^{N} M_{ij} \frac{\partial E_{chem}}{\partial \phi_j} - \sum_{j=1}^{N} M_{ij} \frac{\partial E_{store}}{\partial \phi_j}
\]

where \( n \) represents the number of crystal grains at an arbitrary point. The third term on the right-hand side of Eq. (5) is the phenomenological driving force for the ferrite grain growth. In the case of the DIFT, the magnitude of the driving force, \( \Delta E_{chem} \), is given by the sum of the chemical driving force, \( \Delta E_{chem} \), and the stored energy \( \Delta E_{store} \), as follows:

\[
\Delta E_{chem} = \Delta E_{chem} + \Delta E_{store}
\]

Here, the chemical driving force is described as \( \Delta E_{chem} = \Delta S \Delta T \) at the austenite/ferrite interface, where \( \Delta S \) and \( \Delta T \) are the entropy difference between the ferrite and austenite phases and the extent of undercooling, respectively.\textsuperscript{24} On the other hand, the stored energy is described as

\[
\Delta E_{store} = \frac{1}{2} \mu_{ave} b^2 (\rho_i - \rho_f)
\]

In Eq. (5), \( M_{ij}^s \) is the phase-field mobility, which is related to the physical grain-boundary mobility and the thickness of the austenite/ferrite interface, \( \delta \). For an interface between the ferrite and austenite phases, the phase-field mobility is related to the ferrite/austenite grain-boundary mobility, \( M_{ave} \), as

\[
M_{ave} = \frac{\Delta E_{chem}}{\Delta S \Delta T} = V_f \mu_{ave} + \left(1 - V_f\right) \mu_a
\]

where \( \mu_{ave} \) is the average shear modulus, which is given by a function of the volume fraction of the ferrite phase, \( V_f \), and the shear modulus of the single ferrite phase, \( \mu_a \), and that of the austenite phase, \( \mu_f \), as

\[
\mu_{ave} = V_f \mu_a + \left(1 - V_f\right) \mu_f
\]

The local carbon concentration, \( C \), is defined as a linear function of the local carbon concentration in the \( i \)th grain of the \( \lambda \) (\( \lambda = \alpha \) or \( \gamma \)) phase, \( C_i^\lambda \), weighted by the phase-field variables.\textsuperscript{24,25} The local carbon concen-
tration is given as
\[ c_i^A = \frac{k_i C}{\sum_{j=1}^{n} k_j \phi_j} \].......................... (11)

Here, \( k_i \) is the partition coefficient of the carbon atoms in the \( i \)th grain. Hereafter, for simplicity, we consider an austenite + ferrite two-grain system. Therefore, when \( \phi_1 \) and \( \phi_2 \) correspond to the ferrite and the austenite phases, respectively, the total carbon concentration, \( C \), is written as
\[ C = \sum_{i=1}^{n} \phi_i c_i^A = \phi_1 c_1^A + \phi_2 c_2^A \] ........................ (12)

Using the definition in Eq. (12), the diffusion equation for the total carbon concentration can be expressed by the sum of the diffusion fluxes of carbon atoms from the \( i \)th grain as follows:
\[ \frac{\partial C}{\partial t} = \nabla \cdot \left( \sum_{i=1}^{n} \phi_i D_i \nabla c_i^A \right) \] ........................ (13)

where \( D_i \) is the diffusion coefficient of carbon atoms in the \( i \)th grain. Here, because \( \phi_1 \) and \( \phi_2 \) are the phase-field variables for the ferrite and the austenite phases, \( D_1 \) and \( D_2 \) are the diffusion coefficients of carbon atoms in the ferrite and austenite phases, respectively. The carbon diffusion coefficients in the ferrite and austenite phases are described by the following Arrhenius-type equations:
\[ D_\alpha = D_{\alpha 0} \exp \left( \frac{Q_\alpha}{RT} \right) \] .................. (14)\nand
\[ D_\gamma = D_{\gamma 0} \exp \left( \frac{Q_\gamma}{RT} \right) \] .................. (15)

Here, \( D_{\alpha 0} \) and \( Q_\alpha (i = \alpha \) or \( \gamma \) denote the pre-exponential factor and the activation energy of the carbon diffusion coefficient, respectively.

### 2.2. Modeling of Dislocation-density Evolution and the Flow Stress Curve

In order to simulate the variation in the flow stress during the DIFT, the evolution of the dislocation density owing to plastic deformation was expressed using the Kocks-Mecking (KM) model. The KM model used in this study can be described by the following equation:
\[ \frac{d\rho_i}{d\varepsilon} = k_i \sqrt{\rho_i} - k_j \rho_i \] .................. (16)

The first term of Eq. (16) describes the increase in the dislocation density due to strain hardening. The second term is the decrease in the dislocation density owing to dynamic recovery. \( k_i^\prime \) and \( k_i \) are constants representing hardening and recovery in the \( i \)th grain, respectively. \( k_i^\prime \) is given by
\[ k_i^\prime = \frac{\mu k_i}{2\sigma_i^\prime} \] where \( \sigma_i^\prime \) is the steady-state stress of the \( i \)th grain.

The variation in the flow stress during the DIFT can be calculated using the following equation:
\[ \sigma = \frac{1}{2} \mu \rho_{ave} b \sqrt{\rho_{ave}} \] .......................... (17)

Here, \( \rho_{ave} \) is the average dislocation density in the system and is given as a function of the dislocation density of each grain and the corresponding phase-field variables.

### 2.3. Nucleation of Ferrite Grains during DIFT and DRX

The results of previous experimental studies on ferrite nucleation during the static austenite-to-ferrite transformation in plain carbon steel have shown that ferrite nucleation occurs preferentially on austenite grain boundaries. In the case of the DIFT, the microshear bands and dislocations introduced within the austenite grains by plastic deformation are also potential ferrite nucleation sites. Therefore, we need to describe the nucleation of the ferrite phase both on the austenite grain boundaries and on the microshear bands within the austenite grains.

According to Umemoto et al., during the static austenite-to-ferrite transformation that occurs during continuous cooling, the number of ferrite grains nucleated per unit area of the austenite grain boundary per second can be described as follows:
\[ J_i^g = K_i^g \sqrt{kT} \exp \left( \frac{-K_s^g}{kT} \right) \] ........................ (18)

where the upper index, \( i \), indicates the type of the nucleation site. Here, we take into account two kinds of nucleation sites, that is, those that fall on the grain boundary and the nucleation sites on the microshear bands within the austenite grains. \( J_i^g \) is the diffusion coefficient of carbon atoms in the austenite phase, and \( T \) is temperature of the system. \( k \) is the Boltzmann constant. \( k_i^g \) is a parameter related to the density of the nucleation sites. \( K_g \) is a constant related to the interfacial energy of a ferrite nucleus. Umemoto et al. identified these parameters in order to describe the nucleation of the ferrite phase during the static transformation. However, not only the austenite grain-boundary area, but also the number of active nucleation sites increase owing to the plastic deformation that occurs during the DIFT. Thus, in order to model the increase in the nucleation-site density by the plastic deformation, \( K_i^g \) is phenomenologically described by the following function:
\[ K_i^g = K_i \exp(-\varepsilon) \] ........................ (19)

Here, \( \varepsilon \) represents the strain. The value of \( K_i \) is assumed to be the same as that reported by Umemoto et al. The area of the austenite grain boundary, \( S_{gb} \), is calculated from the length of the austenite grain boundary, \( \ell_g \), which, in turn, is calculated through the MPF simulation as follows:
\[ S_{gb} = \frac{4\ell_g}{\pi} \] ........................ (20)

On the other hand, in order to describe the evolution of the density of the activated ferrite nucleation sites on the microshear band, we determine \( K_i^g \) using the following equation:
\[ K_i^g = K_i \left[ 1 - \exp \left( -\lambda \left( \varepsilon - \varepsilon_{ref} \right) \right) \right] \] ........................ (21)

where \( \varepsilon_{ref} \) is the critical strain for the initiation of microshear band formation and \( \lambda = \dot{\varepsilon} / \varepsilon_{ref} \) is a parameter representing the strain-rate sensitivity of the microshear band formation process. Here, \( \dot{\varepsilon} \) and \( \varepsilon_{ref} \) are the applied strain rate and the referential strain rate, respectively.
increase in the area of the microshear band can be expressed in terms of the following equation:

\[ S' = S_{\text{max}} \left[ 1 - \exp\left\{ - \lambda (\dot{e} - \dot{e}_0) \right\} \right] \] ........................ (22)

where \( S' \) represents the maximum area of the microshear band; this area is assumed to be equivalent to the area of the untransformed austenite phase.

In Eq. (18), \( \Delta G_i \) represents the driving force responsible for ferrite nucleation. It is defined as the sum of the chemical driving force for the nucleation, \( \Delta G_{\text{chem},i} \), and the stored energy, \( G_{\text{store}} \):

\[ \Delta G_i = \Delta G_{\text{chem},i} + G_{\text{store}} \] .......................... (23)

where \( \Delta G_{\text{chem},i} \) is defined as the function of average carbon concentration and temperature that is calculated in accordance with the literatures.\(^{29,30}\) As was the case in Eq. (7), the stored energy can be described as

\[ \Delta G_{\text{store}} = \frac{1}{2} G_{\text{b}} b^2 \rho_{\text{ave}} \] .......................... (24)

The nucleation of ferrite grains that have undergone DRX is assumed to occur on the grain boundaries between pre-formed ferrite grains when the dislocation density in the ferrite grains increases to the critical value, \( \rho_{\text{crit}} \). We employed the following equation to represent the nucleation rate of these ferrite grains:\(^{5,31}\)

\[ \frac{dN_i}{dt} = c \dot{e} \exp \left\{ - \frac{Q}{RT} \right\} \] .......................... (25)

where \( c \) is a parameter characterizing the magnitude of the nucleation rate, \( Q \) is the activation energy for the nucleation of the ferrite grains that have undergone DRX, and \( R \) is the gas constant. Although it has reported that the DRX of austenite can also occur during the DIFT in the case of low-carbon steels, Tong et al.\(^{10}\) found that the DRX of austenite only retards the DIFT slightly. Therefore, the DRX of austenite during the DIFT was not taken into account in this study.

3. Simulation Condition and Procedure

To perform the two-dimensional simulation of the DIFT in a Fe–C binary alloy using the MPF model, the time-evolution equations for the phase-field variable and the carbon concentration were solved using the finite-difference method under the periodic-boundary condition. The simulated domain was discretized using a regular finite-difference grid of \( 512 \times 512 \), which corresponded to a domain of \( 51.2 \times 51.2 \) \( \mu \)m\(^2\). The initial distribution of austenite grains was created by performing a normal-grain-growth simulation. The initial dislocation density in the austenite phase was assumed to be constant at \( 10^7 \) m\(^{-2}\). The diameter of the ferrite nuclei was set to 0.6 \( \mu \)m. The locations of the ferrite nucleation sites on the austenite grain boundaries and those within the austenite grains were selected at random.

In order to determine the input parameters for the MPF model, we performed a preliminary simulation of the DIFT in a Fe-0.15wt.%C alloy at a temperature of 750°C and strain rate of 0.1 s\(^{-1}\); these conditions are same as those employed by Choi et al.\(^{35}\) Then, the parameters to be used for the subsequent MPF simulation were identified by comparing the simulated flow stress curve with the experimentally determined one. The physical values and input parameters obtained using the above-mentioned procedure are shown as follows:\(^{12-20}\) For Eqs. (3) and (4), interfacial energy, \( \gamma_{ij} = 0.5 \) J/m\(^2\) and interfacial thickness, \( \delta = 0.7 \) \( \mu \)m. For Eq. (6), entropy difference, \( \Delta S = 3.46 \times 10^3 \) J/(Km\(^2\)). For Eq. (8), magnitude of the Burgers vector, \( b = 0.25 \) nm, shear modulus of single-phase ferrite, \( \mu_{\alpha} = 32 \) GPa and single-phase austenite, \( \mu_{\gamma} = 50 \) GPa. For Eq. (9), pre-exponential factor of \( M_{\alpha}, M_{\gamma} = 3.5 \times 10^7 \) m\(^2\)/Js, and activation energy \( Q_{\alpha} = 147 \) kJ. For Eq. (10), pre-exponential factor of \( M_{\alpha,\gamma}, M_{\gamma,\alpha} = 1.0 \times 10^7 \) m\(^2\)/Js and activation energy, \( Q_{\alpha,\gamma} = 120 \) kJ. For Eq. (14), pre-exponential factor of \( D_{\alpha}, D_{\gamma} = 4.75 \times 10^{-5} \) m\(^2\)/s and activation energy, \( Q_{\alpha} = 155 \) kJ. For Eq. (15), pre-exponential factor of \( D_{\alpha}, D_{\gamma} = 1.23 \times 10^{-5} \) m\(^2\)/s and activation energy, \( Q_{\alpha} = 99.5 \) kJ. For Eq. (16), we use \( k_{\alpha} = 2.3 \times 10^6 \) m\(^{-1}\), \( k_{\gamma} = 4.5 \times 10^6 \) m\(^{-1}\), \( \sigma_{\alpha}^{*} = 161.1 \) MPa and \( \sigma_{\gamma}^{*} = 315.8 \) MPa. For Eq. (21), constants for the \( \alpha \) nucleation rate, \( f_{\alpha} = 2.07 \times 10^1 \) J/\( \mu \)mol and activation energy, \( Q_{\alpha} = 243.8 \) J/mol. For Eq. (25), we use \( c = 1.0 \times 10^2 \) and \( Q = 170 \) kJ/m\(^2\).

After determining the input parameters, we performed simulations to investigate the effects of the strain rate, the AGS, and the DRX of the ferrite phase on the size of the ferrite grains and the flow stress curve. It should be mentioned that, unless stated otherwise, the temperature, \( T \), was set to 750°C, the strain rate, \( \dot{e} \), to 0.1 s\(^{-1}\), the critical strain, \( \epsilon_{\text{crit}} \), to 0.35, and the austenite grain size, \( d_{\alpha} \), to 5.5 \( \mu \)m.

To determine the size distribution of the ferrite grains formed by the DIFT, the radii of the ferrite grains were calculated as follows:

\[ d_i = 2 \left[ \frac{S_i}{\pi} \right]^{1/2} \] .......................... (26)

where \( S_i \) is the area of the ferrite grain when the phase-field variable corresponding to the ferrite phase was larger than 0.5. Further, the average size of the ferrite grains was calculated as

\[ d_{\text{ave}} = \frac{\sum d_i}{N_{\alpha}} \] .......................... (27)

where \( N_{\alpha} \) is the total number of ferrite grains in the computational domain.

4. Results and Discussion

4.1. Correlation between Flow Stress Curves and Microstructural Evolution

Figure 1 shows the evolution of the flow stress and that of the volume fraction of the ferrite phase with the strain at a deformation temperature of 750°C and strain rate of 0.1 s\(^{-1}\). The volume fraction of the ferrite phase was approximately 0.2. After the peak stress had been reached, significant dynamic softening occurred with an increase in the strain and volume fraction of the ferrite phase. This softening is attributable to the dynamic transformation from the harder austenite phase.
to the softer ferrite phase.

**Figure 2** shows the ferrite grain, carbon-concentration, and dislocation-density distributions for each of the strain levels indicated in Fig. 1. It can be seen that the ferrite grains nucleate preferentially at the austenite grain boundary. At a strain of 0.6, an extremely large number of ferrite grains form on the austenite grain boundary. After the strain reaches the critical value for microshear band formation, which is 0.35, a few ferrite grains nucleate within the austenite grain. The morphology of the simulated microstructure was similar to that observed by Choi et al.\(^3\)\(^2\).

In order to study the effects of plastic deformation on the transformation kinetics and the resulting microstructure, the isothermal transformation was simulated in the absence of the deformation at the same temperature as that used in the case of the simulation corresponding to Fig. 2. The simulated changes in the ferrite grains and that in the carbon concentration during the isothermal transformation are shown in Fig. 3. A comparison of the results shown in Figs. 2 and 3 shows that the DIFT produces a greater number of ferrite grains in a larger volume fraction, because the energy stored owing to the plastic deformation enhances both the rate of nucleation and the growth of the ferrite grains. However, in contrast to the results of experimental studies,\(^3\)\(^2\) the average ferrite grain size after the DIFT was 2.58 μm; this value is slightly larger than that for the isothermal transformation (2.12 μm). One of the reasons for this discrepancy is that the DRX of the ferrite grains was not taken into account in the simulation.

### 4.2. Effect of Critical Strain for Formation of Microshear Band

As Hickson et al.\(^3\) have reported, the nucleation of ferrite grains on the microshear bands formed within austenite grains contributes to the formation of fine-grained ferrite. In this study, we used Eqs. (21) and (22) to describe the nucleation of ferrite grains on the microshear band. In particular, these equations assume that microshear band formation is influenced by the strain rate and the critical strain. Thus, in order to understand the effect of the critical strain on the variation in the flow stress, the DIFT was simulated at low and high strain rates; critical strains, \(\varepsilon_0\), of 0.1, 0.35, and 0.5 were used in the simulations.

**Figure 4(a)** shows the flow stress during the DIFT for a low strain rate (0.1 s\(^{-1}\)). Because the formation of the microshear band is suppressed at a strain rate as low as this, the peak value in the flow stress curve remains unchanged. However, when the critical strain is lower than the strain corresponding to the peak stress, the dynamic softening becomes more pronounced than that in the other two cases. On the other hand, as shown in Fig. 4(b), a number of microshear bands form within the austenite grains at the higher strain rate (0.5 s\(^{-1}\)). This results in an increase in the...
amount of intragranular ferrite formed. Thus, it was found that the flow stress increases with an increase in the critical strain.

4.3. Effect of Strain Rate

To study the effect of the strain rate on the DIFT, we performed simulations using three different strain rates, namely, $\dot{\varepsilon} = 0.05$, 0.1, and 0.5 s$^{-1}$. Figure 5 shows the flow stress curves and volume fractions of the ferrite phase for the different strain rates. It can be seen that the maximum stress decreases with an increase in the strain rate. This is because the time available for the growth of the ferrite grains decreases as the strain rate increases. Therefore, the volume fraction of the ferrite phase also decreases at higher strain rates. It can be seen that, at a strain rate of 0.05 s$^{-1}$, the flow stress slightly increases after the dynamic softening. On the other hand, the flow stress curve corresponding to the DIFT with plastic deformation and a higher strain rate exhibits a single peak, which represents a low degree of softening. These simulated variations in the flow stress with the strain rate are similar to those observed experimentally.9,33)

The evolution behaviors of the ferrite phase at strain rates of 0.05 s$^{-1}$ and 0.5 s$^{-1}$ are shown in Figure 6. At the lower strain rate, the nucleation of the intragranular ferrite is not observed. Furthermore, because there was enough time for the growth of the ferrite grains, the ferrite grains tend to be coarse. When we increase the strain rate, a greater number of microshear bands are formed in the austenite phase. Thus, the nucleation of ferrite grains within the austenite grains is accelerated and very fine ferrite grains are produced.

Figure 7 shows the size distribution of the ferrite grains for a strain of 1.0 and different strain rates. It can be seen clearly that fine-grained ferrite is formed by increasing the strain rate, as has been reported previously.34,35)

4.4. Effect of Austenite Grain Size (AGS)

In order to elucidate the relationship between the AGS
and the ferrite grain size, simulations were performed using three different AGSs. Figure 8 shows the flow stress curves and the volume fractions of the ferrite phase for the different AGSs. As was expected, the number of ferrite nucleation sites increases with a decrease in the AGS. Therefore, the change in the volume fraction of the ferrite phase is higher for smaller AGSs. Furthermore, the occurrence of the hard impingement of the ferrite grains is enhanced by decreasing the AGS. As a result, the maximum value of the flow stress decreases with a decrease in the AGS. The final distributions of the ferrite phase for each AGS are shown in Fig. 9. It can be seen clearly that the ferrite grains decrease in size with the decrease in the AGS. This phenomenon is similar to what has been reported in previous studies. The number and mean diameter of the ferrite grains for the different AGSs are listed in Table 1. As per the microstructure shown in Fig. 9, decreasing the AGS produces a greater number of fine-grained ferrite grains. This suggests that decreasing the AGS is an effective way of obtaining homogeneously distributed, extremely fine ferrite grains; this is in keeping with what has been reported by Beladi et al. 37)

4.5. Effect of DRX of Ferrite Phase

In order to investigate the effect of the DRX of the ferrite phase on the flow stress and microstructural evolution during the DIFT, simulations of the DIFT associated with DRX were performed. It should be mentioned that the interfacial mobility of ferrite subjected to DRX and the critical dislocation density for the DRX of ferrite have not been investigated experimentally. Therefore, we performed the simulations using different mobilities of the grain boundar-
ies of ferrite grains subjected to DRX as well as different critical dislocation densities.

Figure 10 shows the variation in the flow stress and the volume fraction of the ferrite phase during the DIFT corresponding to the DRX for different interfacial mobilities. That is, the grain boundary mobility of the ferrite subjected to DRX, $M_{\alpha/\alpha}$, was changed to 3.0 $M_{\alpha/\alpha}$. It should be noted that the critical dislocation density, $\rho_{\text{cri}}$, was set to $7.2 \times 10^{14}$ m$^{-2}$ for this simulation. The flow stress curves shown in Fig. 10 indicate that the peak stress does not change and that the volume fraction of the ferrite phase increases slightly with an increase in the mobility. As a result, the degree of dynamic softening after the peak stress also increases slightly with the increase in the mobility. Further, as shown in Fig. 11, the morphologies of the microstructures in the two instances are quite different. In both cases, it is observed that small dynamically recrystallized ferrite grains start to nucleate between the preformed ferrite grains at a strain of 0.4. Figure 12 shows a comparison of the histogram of the size of the ferrite grains formed by the DIFT accompanied by DRX and the size of the grains formed by the DIFT in the absence of DRX. When the interfacial mobility is higher, the total number of ferrite grains becomes smaller and coarse ferrite grains are obtained. On the other hand, in the case of a lower interfacial mobility, although the average grain size of the ferrite grains is almost same as that obtained by the DIFT in the absence of the DRX of ferrite, the number of fine ferrite grain less than 2 $\mu$m increases.

Figure 13 shows the simulated variations in the flow stress curve and volume fraction of the ferrite phase for critical dislocation densities of $3.5 \times 10^{14}$ m$^{-2}$ and $1.2 \times 10^{14}$ m$^{-2}$. The final distribution of ferrite grains for both cases is shown in Fig. 14. As shown in Fig. 13, when the mobility of dynamically recrystallized ferrite is higher, the degree of dynamic softening increases slightly, owing to the formation of low-dislocation-density ferrite because of the DRX. However, it is seen that the peak stress and the final ferrite grain size do not change with the change in the critical dislocation density.

The results described in this section suggest that the vari-

![Fig. 11. Evolution of ferrite grains during the DIFT associated with the DRX of the ferrite phase for different interfacial mobilities of the dynamically recrystallized ferrite: (a) $M_{\alpha/\alpha}$ and (b) 3.0 $M_{\alpha/\alpha}$.](image)

![Fig. 12. Size distributions of the ferrite grains formed by the DIFT for different interfacial mobilities of the dynamically recrystallized ferrite grains.](image)

![Fig. 13. Flow stress curves during the DIFT associated with the DRX of the ferrite phase for different critical dislocation densities.](image)

![Fig. 14. Final distributions of the ferrite grains formed by the DIFT for critical dislocation densities of (a) $1.5 \times 10^{14}$ m$^{-2}$ and (b) $3.5 \times 10^{14}$ m$^{-2}$.](image)
ation of flow stress during the DIFT accompanied by DRX can be characterized in terms of the volume fraction of the ferrite phase. It can also be surmised that the interfacial mobility of the dynamically recrystallized ferrite should be small in order to ensure the refinement of the ferrite grains though the DIFT accompanied by DRX. This has been already realized in a number of studies by exploiting the pinning effect of the precipitation particles.38

5. Conclusions

In this study, we employed a MPF model to simulate the microstructural evolution and the variation in the flow stress during the DIFT. Using the MPF model, we performed two-dimensional simulations of the DIFT in a Fe–C alloy. Through the simulations, the effects of the strain rate, the AGS and the DRX of ferrite on the flow stress curve and the ferrite grain size were investigated systematically. The results of the simulations demonstrated that increasing the strain rate and decreasing the AGS were effective ways of producing ultrafine-grained ferrite by the DIFT. The simulation results also suggested that, when the DIFT was associated with the DRX of the ferrite phase, reducing the interfacial mobility of the dynamically recrystallized ferrite was the key to obtaining fine-grained ferrite. These simulated characteristics of the DIFT were in qualitative agreement with those determined through previous experimental and simulation studies. As mentioned in the introduction, the MPF model describes the growth of ferrite grains driven by the curvature of the austenite/ferrite interface in real time better than do MC and CA models. Therefore, it can be said that the investigated MPF model of the DIFT is more useful for simulating the behavior of the DIFT behavior than are other models. However, it should be noted that the results of the simulations performed in this study were evaluated only through qualitative comparisons with previously reported experimental results. In order to allow for quantitatively accurate simulations, the present MPF model will need to be improved. In particular, using crystal plasticity theory, we intended to account for heterogeneous plastic deformation during the DIFT in a future study.

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