A Multi-phase Field Model for Static Recrystallization of Hot Deformed Austenite in a C–Mn Steel

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Received: 5 December 2016 / Revised: 26 March 2017 / Published online: 24 May 2017
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Abstract A multi-phase-field model has been developed to simulate the microstructure evolution and kinetics of the austenite static recrystallization (SRX) in a C–Mn steel. In this model, the bulk free energy that coupling the deformation stored energy with a special interpolation function is incorporated. Both the deformed grain topology and the deformation stored energy have been included in order to investigate the influence of pre-deformation on the subsequent austenite SRX at different hot deformation levels. Diverse scenarios of microstructure evolution show different deformation-dependent recrystallized grain sizes. The transformation kinetics is then discussed by analyzing the overall SRX fraction and the average interface velocity on the recrystallization front.

KEY WORDS: Phase-field; Static recrystallization; Microstructure evolution; Hot deformation; Mesoscopic modeling

1 Introduction

The static recrystallization (SRX) of the austenite is an important physical metallurgy phenomenon in steel industry. It can produce considerable refinement in the austenite grain structures during the controlled rolling processing, which refines the subsequent transformed microstructures of austenite decomposition during the cooling process [1–3]. Owing to its practical importance for the thermo-mechanical processing in steel industry, modeling the SRX microstructures of the austenite has received tremendous attention in variety of steel grades. A large number of empirical models

[4–7] regarding the austenite SRX have been developed to predict the recrystallized grain size and transformation kinetics of recrystallization in hot strip rolling. These models are usually formulated with the quantitative but empirical relationships among the SRX microstructure and the rolling processing parameters, which can in general provide satisfactory predictions about the overall microstructure properties of the austenite SRX. However, they cannot provide a direct view of the microstructure evolution.

Mesoscopic computer simulation provides an alternative approach to study the microstructural phenomenon of recrystallization on the length scale of the microstructure features. Among the various mesoscopic models, the phase-field (PF) method can readily be used to simulate the static recrystallization in metallic materials [8–11]. Zong et al. [8] and Gao et al. [9] had built a PF–SRX model by constructing a special local free energy density, to simulate the recrystallization process after cold rolling in AZ31 Mg alloy. Suwa et al. [10] introduced the misorientation dependences of grain boundary energy and mobility in the phase-field model based on the subgrain growth theory, and investigated the effects of the microstructural

Available online at <http://link.springer.com/journal/40195>.

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inhomogeneities on recrystallization kinetics. Takaki *et al.* [11] took the deformation stored energy into account by the CP-FEM coupling with the multi-phase-field method to simulate the recrystallization process in plastic deformation microstructure. However, majority of these models mainly present capabilities of the developed tools to model the complex microstructural phenomena in the SRX process. There is still further development of phase-field model to more accessibly couple with deformation model to simulate the SRX process in steels.

The object of the present paper is to develop a physically based multi-phase-field model to simulate the microstructural behavior and kinetics of the austenite static recrystallization following hot deformation in a C–Mn steel at the grain scale. Here, both the changes in morphology of the original grains and the stored deformation energy are introduced in order to investigate the influence of pre-deformation on the subsequent austenite SRX at different deformation levels. The attention of this paper is placed on model development specified to both topographic and quantitative depictions of the microstructural phenomena for austenite SRX in carbon steels.

2 Model Concept

2.1 Multi-phase-Field Model

Based on the continuum-field model proposed by Chen [12], a modified multi-phase-field model is developed to describe the microstructure evolution during the static recrystallization of austenite. In this model, phase-field variables η are employed to represent the orientation of each grain. The orientation of the i -th grain is indicated by η_i , which is 1 inside i -th grain, 0 inside other grains and $0 < \eta_i < 1$ within the interface. Then, a set of variables η can be used to define the polycrystalline structures as:

$$\eta = (\eta_1, \eta_2, \eta_3, \dots, \eta_i, \dots, \eta_n). \quad (1)$$

The free energy function F of the system is given by:

$$F = \int_V [f_s + f_e] dV = \int_V \left[m f_0(\eta) + \frac{\kappa}{2} \sum_{i=1}^n (\nabla \eta_i)^2 + f_e \right] dV, \quad (2)$$

where m is the model parameter. κ is the gradient energy coefficient. f_s is the interfacial free energy. $f_0(\eta)$ is the free energy density formulated to be a fourth-order polynomial as below:

$$f_0(\eta_1, \eta_2, \dots, \eta_p) = \sum_{i=1}^n \left(\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2} \right) + \frac{3}{2} \sum_{i=1}^n \sum_{j>i}^n \eta_i^2 \eta_j^2. \quad (3)$$

The bulk free energy f_e is defined by the deformation stored energy E coupled with an interpolation function

$w(\eta)$ at each lattice site. The interpolation function is initially used in modeling the phase transformation in multi-phase systems [13] with a purpose to maintain thermodynamic consistence [13, 14] at the multi-junctions in the calculations.

This interpolation function can be expressed as

$$w_i(\eta) = \frac{\eta_i^2}{\sum_{j=1}^n \eta_j^2}. \quad (4)$$

And the bulk free energy f_e is then given as

$$f_e = \sum_{i=1}^n E_i w_i(\eta). \quad (5)$$

The interpolation function $w_i(\eta)$ describes the volume fraction of the i -th grain at a lattice site. It is assigned to be a value of 1.0 inside i -th grain, but 0 for other grains, which means that the i -th grain has its own stored energy E_i . The bulk free energy then can be expressed by the deformation stored energy in a straightforward way.

Figure 1 illustrates the profile of the phase-field variables η , f_s and $(f_s + f_e)$ across recrystallized and unrecrystallized grains. There is a difference ΔE of the stored energy between recrystallized and unrecrystallized grains, and the bulk free energy f_e can be treated as a mixture of different stored energy E_i on the grain boundaries.

The temporal evolution of the phase-field variable η_i can be calculated by solving the Ginzburg–Landau equation as below [12]:

Fig. 1 Profiles of η and the free energy (f_s , $f_s + f_e$) across the unrecrystallized (UnRex, η_1) and recrystallized (Rex, η_2) grains

$$\frac{\partial \eta_i(r, t)}{\partial t} = -L \frac{\delta F(\eta_1, \eta_2, \dots, \eta_n)}{\partial \eta_i(r, t)}, \quad (6)$$

where L is the kinetic coefficient and t is time. Evolution of η_i follows:

$$\frac{\partial \eta_i}{\partial t} = -L \left[m \frac{\partial f_0(\boldsymbol{\eta})}{\partial \eta_i} - \kappa \nabla^2 \eta_i + \frac{\partial (\sum_i E_i w_i(\boldsymbol{\eta}))}{\partial \eta_i} \right]. \quad (7)$$

The model parameters L , κ and m are related to the grain boundary energy σ_{gb} , the mobility μ_{gb} and the interface thickness δ as follows [15]:

$$\kappa = \frac{3}{4} \sigma_{gb} \delta, m = 6 \frac{\sigma_{gb}}{\delta}, L = \frac{4}{3} \frac{\mu_{gb}}{\delta}. \quad (8)$$

The grain boundary mobility μ_{gb} is related with the grain boundary self-diffusion coefficient, D_0 , the activation energy for grain boundary motion, Q_m , and the temperature, T , that can be calculated by [16].

$$\mu_{gb} = \frac{D_0 b^2}{kT} \exp\left(-\frac{Q_m}{RT}\right), \quad (9)$$

where b is the magnitude of the Burger's vector, R is the gas constant and k is the Boltzmann constant ($1.38 \times 10^{-23} \text{ J K}^{-1}$).

2.2 SRX Nucleation Model

Nucleation of austenite SRX can be thought as a thermally activated process. In this study, nucleation of SRX is assumed to only occur at the grain boundaries. The nucleation rate $\dot{N}$ is given by using the following phenomenological relation [16, 17]:

$$\dot{N} = C_0 (E - E_c) \exp(-Q_a/kT), \quad (10)$$

where Q_a is the activation energy for nucleation. C_0 is a fitting constant. E is the deformation stored energy and E_c is the critical energy for triggering recrystallization in the deformed microstructure, which can be derived from the critical deformation strain [17].

$$E_c = \sigma_{gb} \cdot 10^7 \left(\frac{\varepsilon_c}{2.2\varepsilon_c + 1.1} \right), \quad (11)$$

where the critical strain ε_c is generally in the range from 0.05 to 0.1. For the studies on deformation and recrystallization of C–Mn steel, the critical strain can be set to 0.1.

2.3 Calculation of the Stored Deformation Energy

During hot deformation, part of the deformation energy is stored in the form of dislocations. However, in order to evaluate the deformation stored energy E , a number of assumptions must be made regarding the dislocation arrangement in the deformation substructure. Then the

deformation stored energy E can be calculated using two principal parameters, the free dislocation density (ρ) and the subgrain diameter (δ_{sub}) [18]:

$$E = \frac{1}{2} G b^2 \rho + \frac{3\sigma_{sub}}{\delta_{sub}}, \quad (12)$$

where G is the shear modulus and σ_{sub} is the sub-boundary interfacial energy (0.2 J m^{-2}). The relationship between the flow stress σ and the dislocation density ρ can be expressed as follows [19]:

$$\sigma = \alpha G b \sqrt{\rho}, \quad (13)$$

where α is a dislocation interaction term which is 0.5 for most metals.

Here, the evolution of flow stress σ with strain ε and strain rate $\dot{\varepsilon}$ during the hot deformation is adopted as follows [20]:

$$\sigma = (A\varepsilon^{n_1} - B\dot{\varepsilon}) \exp\left(\frac{Q_{def}}{RT}\right), \quad (14)$$

where A , B , n_1 and n_2 are the fitting parameters related to the material composition. Q_{def} is the deformation activation energy. Values of the above fitting parameters for σ prediction are presented in Table 1. Figure 2 shows the predicted stresses at different strains compared with that from the experimental measurements in the same steel grade [7, 21, 22] under the given deformation condition of $T = 900^\circ\text{C}$ and $\dot{\varepsilon} = 1.0 \text{ s}^{-1}$. It can be seen that the flow stress increases with the strain increasing. The predictions agree well with the experimental results, indicating a good availability of the model. Thus, it can be used reasonably to calculate the deformation stored energy in this steel grade.

3 Simulation Settings

The investigated steel in this study is a plain C–Mn steel with a composition of 0.1C–1.3Mn–0.2Si (mass%). The SRX microstructure behavior, which occurs after a uniaxial compression deformation up to a series of logarithmic strains of $\varepsilon = 0.2, 0.3, 0.4$ and 0.5 , is considered under a strain rate of $\dot{\varepsilon} = 1.0 \text{ s}^{-1}$ at a fully austenitic temperature of $T = 900^\circ\text{C}$. The values of the input parameters used in the model are presented in Table 2.

The input undeformed microstructure is discretized with a 300×400 lattice space representing a physical domain of $120 \mu\text{m} \times 160 \mu\text{m}$ with 96 polygonal austenite grains

Table 1 Values of the fitting parameters for σ prediction

n_1	n_2	A	B	Q_{def} (kJ mol ⁻¹)
0.45	0.1	48	30	22

Fig. 2 Flow stresses as functions of strain during hot rolling at $T = 900\text{ }^{\circ}\text{C}$ and $\dot{\varepsilon} = 1.0\text{ s}^{-1}$ for C–Mn steels. The model prediction compares with experimental measurements

as shown in Fig. 3. The initial average grain size of the austenite grains is about $16\text{ }\mu\text{m}$ in diameter. However, the grain topology will change due to the different deformation levels, which is also an important input for subsequent SRX simulations. Here, the grain deformation is modeled by combination with a topology deformation approach based on a vector operation [20]. In a 2D model, the topology deformation can be described by a 2×2 deformation matrix. Thus, an original vector $\mathbf{u}$ becomes a new vector $\mathbf{v}$ as a result of a uniform deformation S .

$$\mathbf{v} = S\mathbf{u}. \quad (15)$$

The form of matrix can be written as

$$\begin{bmatrix} v_x \\ v_y \end{bmatrix} = \begin{bmatrix} S_x & 0 \\ 0 & S_y \end{bmatrix} \begin{bmatrix} u_x \\ u_y \end{bmatrix}, \quad (16)$$

where $u_i (i = x, y)$ are the components of original vector $\mathbf{u}$ and $v_i (i = x, y)$ are the components of new vector $\mathbf{v}$ after deformation. $S_i (i = x, y)$ are the principal nominal deformation at the two directions (the ratios of the final to initial lengths of vectors along two principal axes). Therefore, $\varepsilon_i = \ln S_i (i = x, y)$ are the true strains along the two principal axes of deformation. And the determinant of S must be unity so as to remain the volume unchanged, i.e., $S_x S_y = 1$. The geometrical change of each cell due to the deformation can be determined. In this way, the grain deformation due to the deformation can be simulated when the pre-strain is imposed on the entire lattice.

Fig. 3 Initial undeformed microstructure

After a series of pre-strains of $\varepsilon = 0.2, 0.3, 0.4$ and 0.5 , the initial regular lattice is changed to be 296×404 , 242×494 , 219×546 and 179×667 , respectively. The initial microstructure is compressed in the longitudinal direction and elongated normal to the compressed direction, and there is an obvious increase in the total grain boundary areas as seen in Fig. 4. The changes in the morphology of the deformed grain will influence the subsequent nucleation and grain growth in the microstructure evolution and the kinetics.

Details regarding to the numerical implementation of the MPF method in simulating the microstructure evolution, the reader can refer to the literatures [13, 15]. Here, only the items relevant to the current simulation are listed in more detail:

1. The initial polycrystalline structure is achieved by the general grain growth.
2. The deformed grain topology and the deformation stored energy under different strains in the uniform system are obtained by the deformation model.
3. The continuous nucleation method is employed and the nuclei are only distributed on the grain boundaries. The radius of the nuclei is set to be $3\Delta x$. Once a nucleation takes place at a site, a new phase-field variable η_{n+1} (equals to 1.0) will be used to mark this new grain, and other phase-field variables take the value of 0 in this grain interior. This process will last until all potential sites are examined at each time step.
4. The phase-field equations are solved numerically by a finite difference discretization with explicit time stepping.

Table 2 Key parameters used in simulations [16]

G (GPa)	b (m)	Q_m (kJ mol $^{-1}$)	σ_{gb} (J m $^{-2}$)	D_0 (m 2 s $^{-1}$)	Q_a (kJ mol $^{-1}$)
80	2.48×10^{-10}	140	0.56	1.1×10^{-13}	170

Fig. 4 Increase in grain boundary area with increasing strain ε . S_0 is the original grain boundary area and S_d is the grain boundary area after deformation

- For the numerical stability and convergence, the interface thickness δ equals to $6\Delta x$ and the time step Δt is related to the grid spacing Δx , $\Delta t < \Delta x^2/4u_{gb}$.

4 Results and Discussion

4.1 SRX Microstructure Evolutions

Figure 5 shows the microstructure evolution of the austenite during SRX at different strains of $\varepsilon = 0.2, 0.3, 0.4$ and 0.5 .

The figures show the SRX nucleation and growth process in the hot deformed matrix, in which the black lines represent the grain boundaries, the gray areas represent the original deformed grains and the areas in different colors are the recrystallized grains with different crystallographic orientations. It can be seen that the obvious refinement in the SRX grains realize with the increasing pre-strains. According to the aforementioned analysis, increasing the pre-strain can provide a high level in the stored deformation energy, which hence leads to a higher nucleation rate of the SRX. As a result, a larger SRX nucleation density is produced at the higher deformation level. On the other hand, increasing deformation causes a topological change with compression in the vertical direction and an elongation normal to the compression direction. The change in grain topology with increasing deformation leads to a remarkable increase in the total grain boundary areas, which provides more nucleation sites for the SRX nuclei. As a consequence, obvious grain refinement is observed with the increased deformation as seen in Fig. 5.

Figure 6 shows the change of the recrystallized grain number during the SRX at different pre-strains. It can be seen that larger pre-deformation produces much more recrystallization grains during the SRX. The number of SRX nuclei is found to increase rapidly at the early stage of the SRX till the nucleation sites become saturated, and then decrease gradually with the SRX proceeding. It is specially obvious at the higher deformation level as shown in Fig. 6. During the SRX, nucleation occurs preferably and continuously at the initial grain boundaries. The SRX nuclei then

Fig. 5 Simulated microstructural evolution during the austenite SRX after hot deformation under different pre-strains of **a** $\varepsilon = 0.2$, **b** $\varepsilon = 0.3$, **c** $\varepsilon = 0.4$, **d** $\varepsilon = 0.5$

Fig. 6 Variations of the SRX grains number with time under different pre-strains

grow up gradually consuming the original deformed grains including the preferred nucleation size at the grain boundaries. At a higher pre-deformation, the larger stored energy leads to much higher nucleation density. Meanwhile, a decrease in the spaces between the grain boundaries along the vertical direction is observed and hence provides short distances for the growth of the individual recrystallized grains nucleated on the grain boundaries. New SRX nuclei readily impinge on each other and the subsequent grain coarsening due to the grain boundary energy is promoted, which thus leads to further vanishing of the recrystallized nuclei during the SRX process.

Figure 7 shows the corresponding changes of the average size of the recrystallized grains at different strains. In this paper, the mean grain size is defined by the average grain sphere diameter d_{aver} as follows:

$$d_{\text{aver}} = \frac{\sum_{i=1}^N \sqrt{\frac{A_i}{\pi}}}{N}, \quad (17)$$

where A_i is the area occupied by the recrystallized grain i , and N is the total number of the recrystallized grains. It clearly shows that the average size of SRX grains increases faster at the early stage of the SRX at a higher pre-deformation level, but the final recrystallized grains is much finer. The resultant grain sizes are 14.5, 11.2, 9.8 and 8.6 μm at the pre-strains of $\varepsilon = 0.2, 0.3, 0.4$ and 0.5 , respectively. It is clearly indicated the grain refinement of the SRX due to the increasing pre-deformation level.

As an important physical metallurgical transformation closely correlated with the hot strip rolling in steel industry, the grain size of austenite SRX can also be predicted by the macroscopic empirical microstructural models. The macroscopic models are usually formulated concerning the quantitative but empirical relationships among the

Fig. 7 Average SRX grain size d_{aver} as a function of time under different pre-strains

microstructures and the processing parameters for a given steel grade based on a large amount of experimental data available from laboratory simulations [1, 3, 23]. For this steel grade, the recrystallized grain size of the austenite, d_{rex} , after complete recrystallization can be predicted by an empirical model [6, 7]:

$$d_{\text{rex}} = A d_{\gamma}^q \varepsilon^{-p} \exp(-Q_{\text{gx}}/RT), \quad (18)$$

where A , q , p and Q_{gx} are fitting parameters depending on the steel grade investigated [6, 7]. Based on grain boundary nucleation of SRX, $q = 1/3$ is proposed to describe the effect of the initial austenite grain size d_{γ} [24]. And the effect of pre-strain is captured with value of p that fall into the range $1/3$ – 1 in the C–Mn steel grade [3, 6]. In this PF simulation, a value of $p = 0.56$ is proposed as seen in Fig. 8 which is rationalized in the investigated steel. It is indicated that this MPF model of austenite SRX can replicate the grain refinement due to increasing the pre-strains in SRX process.

4.2 SRX Kinetics

The SRX kinetics at different strains is shown in Fig. 9. It is clearly seen that the time for 50% recrystallization, $t_{0.5}$, decreases with increasing the pre-strains, which indicates a faster SRX transformation kinetics due to increasing deformation. In general, the recrystallization kinetics can be described using the well-known JMAK approach [6, 7]:

$$F_{\text{rex}} = 1 - \exp(-0.693(t/t_{0.5})^{n_{\text{rex}}}), \quad (19)$$

where F_{rex} is the fraction recrystallized, n_{rex} is the Avrami exponent and $t_{0.5}$ is the time for 50% recrystallization. For SRX, $t_{0.5}$ can be expressed as a function of initial austenite grain size d_{γ} , strain ε , strain rate $\dot{\varepsilon}$ and temperature T and given by [6, 7]:

Fig. 8 Average grain size $\ln(d_{\text{rex}})$ with the respect to $\ln \varepsilon$

Fig. 9 Simulated SRX kinetics under different pre-strains and a comparison with the predictions by the JMAK model

$$t_{0.5} = C d_{\text{r}}^{c_1} \varepsilon^{c_2} \dot{\varepsilon}^{c_3} \exp\left(\frac{Q_{\text{rex}}}{RT}\right), \quad (20)$$

where the parameters C , c_1 , c_2 and c_3 have to be obtained from the experiments. Using the format of this empirical equation, $\ln t_{0.5}$ is plotted against $\ln \varepsilon$ at the given deformation condition in Fig. 10. It appears to be a linear-like, which indicates a reasonable description about the influence tendency of the strain on the SRX kinetics.

The results in Fig. 9 indicate that the PF simulations are coincident with the JMAK predictions with the Avrami exponent of $n_{\text{rex}} = 1.3$ which falls into a reasonable range 1–2 based on the heterogeneous SRX nucleation [6, 7, 25, 26]. However, significant deviation does still exist between them, especially under the circumstance of lower deformation level. It should be noted that the JMAK theory has assumed an ideal scenario with homogeneous nucleation and isotropic growth of spherical grains, which is rather an exception in real transformations [6]. In the PF

Fig. 10 Relation between $\ln t_{0.5}$ and $\ln \varepsilon$

simulation, however, continuous SRX nucleation at the grain boundaries has been assumed, which introduces obvious heterogeneous nature of the transformations. At the lower pre-strains, the lower nucleation rate has produced less SRX nuclei at the early stage which hence leads to slower transformation kinetics. With increasing of the SRX nuclei as well as their continuous growing, the transformation kinetics becomes much faster at the late stage of the SRX compared with the JMAK predictions. At the higher pre-strain, the higher nucleation density leads to similar condition of homogeneous nucleation and isotropic growth which is much consistent with the JMAK assumptions. Then, the PF results agree well with the JMAK predictions under this circumstance, as seen in Fig. 8. Nevertheless, PF simulation has considered a clear nucleation and growth scenario during the SRX process. It can easily give time- and space-dependent descriptions of the transformation processes. Therefore, the PF method can be easily used to simulate more realistic transformation behaviors than the JMAK theory does.

The SRX kinetics can also be discussed by analyzing the recrystallization front as shown in Fig. 11. Here, the average velocity of the recrystallization front $\langle v \rangle$ is calculated by using the Cahn–Hagel relation [27]:

$$\langle v \rangle = \frac{1}{S_v} \frac{dF_{\text{rex}}}{dt}, \quad (21)$$

where S_v denotes the total area of the recrystallization front per unit volume, which is also termed as *microstructural path* [28, 29]. In a 2D simulation, S_v is replaced by the total length of the recrystallization front per unit area. It can be seen that the velocity of the recrystallization front increases markedly with increasing the deformation level. Nevertheless, it decreases gradually at the final SRX stage. The velocity decreases more abruptly for the higher strain due to the prosperous impingement among the recrystallized grains. As expected, the PF model makes a good

Fig. 11 Average interface velocity $\langle v \rangle$ as a function of time

representation of the microstructural behavior of the SRX. It is also indicated that, apart from the JMAK theory, the Cahn–Hagel relation provides an alternative method to describe the complexity of SRX kinetics since it takes fully into account of the impingements of the recrystallized grains.

5 Conclusions

A multi-phase-field model has been developed to simulate the microstructure evolution and kinetics of the austenite SRX in a C–Mn steel. In this model, both the influences of the deformed grain topology and the deformation stored energy have been considered. The main conclusions are summarized as follows:

By comparison with the macroscopic empirically based SRX model, the physically based MPF modeling of the microstructures can offer a better insight into how the microstructure evolution occurs. It can readily provide time- and space-dependent descriptions of the microstructural process and transformation kinetics of SRX.

As a result of the PF-SRX simulation, the refinement of the recrystallized grains derived from the increasing pre-deformation level can be well replicated based on the microstructural scenario of nucleation and growth. The PF-SRX model also presents a reasonable description about the overall SRX kinetics under different pre-deformations as well as the growth kinetics with respect to the recrystallization front. The PF-SRX model can be readily

used to simulate more realistic SRX behaviors in carbon steels.

Acknowledgements This work was financially supported by the National Science Foundation of China (Grant No. 51371169) and (Grant No. 51401214).

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