Cellular automaton simulation of ferrite-austenite transformation in low-carbon steels

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Abstract. A two-dimensional (2-D) cellular automaton (CA) model is adopted to simulate ferrite (α)-austenite (γ) transformation in low-carbon steels. In the model, the preferential nucleation sites of austenite, the driving force of phase transformation coupled with thermodynamic parameters, solute partition at the α/γ interface, and carbon diffusion in both the α and γ phases are taken into consideration. The model is able to simulate the ferrite-to-austenite transformation during isothermal heating in the ferrite-austenite two-phase region, and the austenite-to-ferrite transformation during continuous cooling. The influences of cooling rate and α grain size on the final carbon concentration field are investigated. The results show that after isothermal heating at 815°C for 300 s, the carbon concentration in both the α and γ phases reach the respective equilibrium values. The simulated microstructures compare well with the SEM images. After cooling to room temperature, the carbon distribution is more uniform when cooled at 1.2°C/s than at 7°C/s. The carbon distributions for different α grain sizes cooled at 1.2°C/s are similar. The simulation results are used to understand the mechanisms of the experimental phenomena of an enameling steel.

1. Introduction

In addition to the casting process, the subsequent heat treatment also impacts significantly the microstructures of the casted metal materials, and thereby the final mechanical properties. It is therefore necessary to study the phase transformation during different heat treatment processes. Among these transformations, ferrite-austenite transformations occupy a significant position in current research because of their fundamental role in solid-solid phase transformations. Extensive experimental work [1-5] has been carried out to study the mechanisms of ferrite-austenite phase transformation. Due to the limitation of the analytical tools, however, the microstructure evolution and solute distribution during solid-solid phase transformation could hardly be observed in real-time.

With the recent development of numerical models, simulations using different methods, such as the phase field (PF) method [6,7], the Monte Carlo (MC) method [8,9] and the cellular automaton (CA) method [10-13], can provide insight into the microstructure evolution and solute diffusion during the ferrite-austenite transformation. The present authors proposed a two-dimensional (2-D) CA model to simulate the ferrite (α)-austenite (γ) transformation and carbon diffusion during different heat treatment processes [14]. In this paper, the previously proposed CA model is applied to simulate the evolution of microstructure and carbon concentration field during continuous cooling with different
cooling rates after isothermal heating in the ferrite-austenite two-phase region. The influence of cooling rate and \(\alpha\) grain size on the carbon distribution is investigated. The simulation results are used to understand the mechanisms of the experimental phenomena that a cold-rolled low-carbon enameling steel exhibits different mechanical properties after different heat treatment processes.

2. Experimental phenomena

The material used in the experiment is a hot-rolled enameling steel, containing 0.07 wt.% C, 0.43 wt.% Si, 1.22 wt.% Mn, 0.04 wt.% P, and 0.001 wt.% S, produced by thin-slab continuous casting and direct hot rolling. The steel was then subject to the heat treatment processes, including isothermal heating at 815°C for 5 min and subsequent air cooling (~7°C/s) or sand cooling (~1.2°C/s). Other samples with the same composition as listed above, but having different grain sizes produced by different rolling processes were sand cooled after heated at 815°C for 5 min to investigate the influence of the \(\alpha\) grain size on mechanical properties.

Figure 1 presents the stress-strain curves of samples with a similar average \(\alpha\) grain size of about 7 \(\mu\)m after isothermal heating at 815°C for 5 min and then cooled by air cooling and sand cooling. As shown, the sample sand cooled has a higher yield strength but a lower tensile strength compared to the sample air cooled. In addition, the yield platform of the sample sand cooled is longer and more obvious than that of the sample air cooled.

Figure 2 shows the stress-strain curves of samples with different \(\alpha\) grain sizes after isothermal heating at 815°C for 5 min and then cooled by sand cooling. The sample with the finer \(\alpha\) grain size exhibits both higher yield strength and tensile strength compared to the sample with the coarser \(\alpha\) grains. However, the yield platforms of the both samples are similar.

It is known that the yield platform is closely related to the Cottrell atmospheres, and the sufficient carbon diffusion contributes to the formation of the Cottrell atmospheres. Therefore, a previously proposed CA model [14] is applied to simulate the \(\alpha\)-\(\gamma\) transformation and carbon diffusion during different heat treatment processes to verify the mechanisms of the experimental phenomena exhibited in figures 1 and 2.

3. Model description and numerical algorithm

The experimental material is a multi-component Fe alloy. For simplicity, a pseudo-binary Fe-C alloy is adopted in the present simulations. The initial carbon concentration used in the simulation is taken as \(u_0 = 0.375\) mol.% C. This composition will produce the equilibrium \(\gamma\) phase fraction of 0.327 at 815°C, which is identical with that of the experimental steel. The phase transformations of both \(\alpha\rightarrow\gamma\)
during isothermal heating and $\gamma \rightarrow \alpha$ during cooling are simulated, while the coarsening of ferrite grains is neglected. The heat treatment processes used in the simulations are divided into two parts:

(1) Isothermal heating: The heating temperature is 815°C and holding time is 300 s. During isothermal heating, $\alpha \rightarrow \gamma$ phase transformation, solute carbon partition at the $\alpha/\gamma$ interfaces, and carbon diffusion in both the $\alpha$ and $\gamma$ phases take place;

(2) Continuous cooling from 815°C to room temperature: The temperature decreases from 815°C to room temperature at the cooling rates of 1.2°C/s and 7°C/s, corresponding to sand cooling and air cooling, respectively. During cooling, $\gamma \rightarrow \alpha$ phase transformation, carbon partition at the $\alpha/\gamma$ interfaces, and carbon diffusion take place. In the present model, the phase transformation of austenite to pearlite is not considered. Considering the kinetic effect on phase transformation, the end temperatures of $\gamma \rightarrow \alpha$ phase transformation are taken as 650°C and 600°C for the cooling rates of 1.2°C/s and 7°C/s, respectively. When the temperature is cooled down below the end temperature, the retained austenite is assumed to be transformed to supersaturated ferrite, while carbon diffusion continues to room temperature.

According to the interface dynamic theory [15] and the assumption of dilute solution, the velocity of interface migration, $v_n$, is calculated by

$$v_n = M_{eff} \left\{ -RT_M \left( k_e - 1 \right) \left[ u^\alpha(T) - u^\gamma(T) \right] / V_m \right\} \tag{1}$$

where $V_m$ is the molar volume, $R$ is the gas constant, $M_{eff}$ is the interface mobility, $T_M$ is the allotropic transformation temperature, $u^\alpha(T)$ is the actual carbon concentration in ferrite at temperature $T$, and $k_e$ is the equilibrium partition coefficient, defined as $k_e = u_e^\gamma(T) / u_e^\alpha(T)$, where $u_e^\alpha(T)$ and $u_e^\gamma(T)$ are the equilibrium concentrations in ferrite and austenite at temperature $T$, respectively. The relevant thermodynamic data are obtained from the phase diagram calculation using Pandat [16], a thermodynamic phase diagram calculation software. Equation (1) indicates that the interface velocity $v_n$ is determined by both the interface mobility $M_{eff}$ and the local concentration difference $u^\alpha(T) - u^\gamma(T)$, where $u^\alpha(T)$ is determined by carbon diffusion.

The interface mobility, $M_{eff}$, is calculated by [17]

$$M_{eff} = M_0 \exp \left( -Q / RT \right) \tag{2}$$

where $M_0$ is the pre-exponential factor, $Q$ is the activation energy. In the present model, the value of $M_{eff}$ is taken as $4.2 \times 10^7 \exp(-14700/RT) \text{ m}^2/\text{s} \cdot \text{J} [18]$.

During ferrite-austenite phase transformation, solute partition at the $\alpha/\gamma$ interfaces is considered according to $u^\gamma = k_{ue} u^\alpha$. Defining the mean carbon concentration as $u = \phi u^\alpha + (1-\phi) u^\gamma$, where $\phi$ is the $\alpha$ phase fraction, carbon diffusion in 2D is calculated by

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left[ D(\phi) \frac{\partial u^\alpha}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D(\phi) \frac{\partial u^\alpha}{\partial y} \right] \tag{3}$$

where $D(\phi)$ is the diffusion coefficient associated with the fraction of ferrite, calculated by

$$D(\phi) = \phi D^\alpha + k_e (1-\phi) D^\gamma \tag{4}$$

where $D^\alpha$ and $D^\gamma$ are the carbon diffusivities in the $\alpha$ and $\gamma$ phases, equaling $2.2 \times 10^{-4} \exp(-122500/RT) \text{ m}^2/\text{s}$ and $1.5 \times 10^{-5} \exp(-142100/RT) \text{ m}^2/\text{s}$ [6], respectively.

In the present CA model, the computational domain is divided into a lattice of $236 \times 348$ square cells with cell size of $\Delta x = 0.3 \mu m$, corresponding to a real domain of $72 \mu m \times 105 \mu m$. Each cell is characterized by the following variables: (1) grain orientation, $I$; (2) $\alpha$ phase fraction, $\phi$ (the cell represents the $\alpha$ phase or $\gamma$ phase, when $\phi = 1$ or $\phi = 0$, respectively); (3) the symbol $\phi_{int} = 1$ indicates the cells at the $\alpha/\gamma$ interfaces; and (4) mean carbon concentration, $u$. The solution sequence for the simulation is as follows: (1) assign the initial state for each cell; (2) track $\alpha/\gamma$ interface and calculate
the increment of ferrite fraction for the interface cells; (3) update the states of all cells in each time step; (4) calculate carbon diffusion in both the $\alpha$ and $\gamma$ phases; (5) repeat steps (2)-(4) for the different heat treatment processes. The time step is determined by $\Delta t = \Delta x^2/4.5D^\alpha$, and the zero-flux boundary condition is adopted. Other details about the implementation of the numerical algorithms used for the simulations of phase transformations and carbon diffusion can be found elsewhere [14].

4. Results and discussion

4.1. Effect of cooling rate

At the beginning of the simulation, the computational domain is initialized with a uniform carbon concentration $u = u_0$ and $\alpha$ grains with various grain orientations. The number of initial $\alpha$ grains is taken as 112 according to the metallography, corresponding to the average $\alpha$ grain size of 6.9 $\mu$m. Based on the experimental observations, the nucleation sites of austenite are preferentially distributed at the ferrite grain boundaries.

During the isothermal heating at 815°C, $\alpha \rightarrow \gamma$ phase transformation and carbon diffusion takes place. Figure 3 (a) shows the simulated $\gamma$ phase fraction varying with time. At the early stage of $\alpha \rightarrow \gamma$ transformation, the increasing velocity of $\gamma$ phase fraction is slow. Then, the $\gamma$ phase fraction increases evidently within 0.1 s~10 s, which implies that the $\alpha \rightarrow \gamma$ transformation might take place mainly during this period. After holding about 11 s, the $\gamma$ phase fraction approaches gradually the equilibrium value of 0.327. Figure 3 (b) shows the simulated mean carbon concentrations in the $\alpha$ phase and $\gamma$ phase varying with time. As shown, in the early stage around $t < 0.4$ s, the mean carbon concentration in the $\alpha$ phase decreases dramatically. This is because the carbon solubility in the $\alpha$ phase is lower than that in the $\gamma$ phase. During the $\alpha \rightarrow \gamma$ phase transformation, carbon partition at the $\alpha/\gamma$ interface takes place. The carbon concentration in the $\alpha$ phase decreases dramatically. This is because the carbon solubility in the $\alpha$ phase is lower than that in the $\gamma$ phase. The carbon concentration in the $\alpha$ phase is absorbed by the formed $\gamma$ phase. After around $t > 1$ s, the carbon concentration in the $\alpha$ phase gradually approaches the equilibrium value of 0.0082 mol.%. On the other hand, the variation of the mean carbon concentration in the $\gamma$ phase exhibits a different trend. At the beginning, the mean carbon concentration in the $\gamma$ phase increases with time and reaches the maximum value of 10.48 mol.% when the time is around 0.03 s. Then, it decreases remarkably. After around 10 s, the carbon concentration in the $\gamma$ phase approaches the equilibrium value of 1.13 mol.%. The increase of the carbon concentration in the $\gamma$ phase at the early stage could be explained by the competition between phase transformation rate and carbon diffusion. At the early stage of the $\alpha \rightarrow \gamma$ transformation, the phase transformation rate is slow as indicated in figure 3 (a). The rate of carbon diffusion from the $\alpha$ phase to the $\gamma$ phase is higher than the growth rate of the $\gamma$ phase, leading to the mean carbon concentration in the $\gamma$ phase increasing in this period.

![Figure 3](a) (b)

**Figure 3.** Time history of (a) $\gamma$ phase fraction, and (b) mean carbon concentration in $\alpha$ and $\gamma$ phases.
Figure 4 (a) presents the simulated carbon concentration field of an Fe-0.375 mol.% C alloy after isothermal heating at 815°C for 300 s. The regions of the high and low carbon concentration are the γ phase and α phase, respectively. It is noted that the carbon concentrations are nearly uniform in the both α and γ phases and reached their respective equilibrium values. Figure 4 (b) shows the SEM image obtained by quenching the experimental sample after heating at 815°C for 300 s to retain the austenite morphology. It is noted that the simulated morphology of austenite grains is somewhat coarser than that observed experimentally, which might be due to the following two main reasons. The current CA model adopts the instantaneous nucleation model for austenite nucleation, while austenite might nucleate continuously during the experimental ferrite-austenite transformation. In addition, the simulation is performed in a 2-D domain, while the dimensionality in the sample is 3-D. Nevertheless, the simulated microstructure agrees reasonably with the experimental observation.

![Figure 4](image)

**Figure 4.** (a) Simulated carbon concentration field and (b) SEM image of an Fe-0.375 mol.% C alloy after isothermal heating at 815°C for 300 s, and then quenching.

Figure 5 presents the evolution of the carbon concentration field of an Fe-0.375 mol.% C alloy during cooling at 1.2°C/s after isothermal heating at 815°C for 300 s. The lower 8 levels and the upper 5 levels of the color legends show the carbon concentrations in the α and γ phases, respectively. According to the model assumption, for the slow cooling rate, γ→α transformation and carbon diffusion take place when the temperature is above 650°C, while only carbon diffusion is considered between 650°C to room temperature. As shown in figures 5 (a) and (b), the carbon concentration is higher in the areas adjacent to the α/γ interfaces, due to the fact that the newly formed α phase rejects carbon atoms during the γ→α transformation. Driven by the concentration gradients, carbon diffusion occurs in both α and γ phases. When the temperature decreases to 650.1°C (figure 5 (c)), the carbon distribution in the ferrite matrix appears to be nearly uniform, indicating that the rate of carbon diffusion in ferrite is sufficient due to the slow γ→α transformation with a low cooling rate of 1.2°C/s. Then, the small quantity of the retained austenite is transformed to be the supersaturated ferrite and carbon diffusion continues. When cooled to room temperature, the carbon concentration field is nearly uniform as shown in figure 5 (d). The maximum and minimum concentrations are 0.375 mol.% C and 0.374 mol.% C, respectively, indicating a sufficient carbon diffusion when cooled at 1.2°C/s.

Figure 6 presents the evolution of the carbon concentration field of an Fe-0.375 mol.% C alloy during cooling at 7°C/s after isothermal heating at 815°C for 300 s. In this case the end temperature of γ→α transformation is assumed to be 600°C. Comparing figures 6 (a) and (b) with figures 5 (a) and (b), it is found that at the similar temperatures during cooling, the fraction of retained austenite is higher and the carbon concentration in ferrite is less uniform for the case of 7°C/s than for the case of 1.2°C/s. Figure 6 (c) shows the carbon concentration field when the temperature reaches 602.3°C. The high concentration regions distributed at grain boundaries illustrate the retained austenite that is transformed to the supersaturated ferrite when the temperature is below 600°C. Then, carbon diffusion continues as the temperature is further decreased to room temperature. The maximum and minimum carbon concentrations at room temperature obtained from cooling at 7°C/s are 2.845 mol.% C and 0.279 mol.% C, respectively. Comparing figure 5 (d) with figure 6 (d), it is obvious that the carbon concentration field cooled at 1.2°C/s is more uniform than that cooled at 7°C/s. Apparently, the cooling process with lower cooling rate provides more sufficient time for carbon diffusion, which is beneficial for carbon diffusion to the locations of dislocations to form high concentration Cottrell
atmospheres. It is known that high concentration Cottrell atmospheres contribute to pinning dislocations, leading to an obvious yield platform in the stress-strain curve, and an increased yield strength [3]. However, Cottrell atmospheres have less effect on the tensile strength and the tensile strength could be increased by increasing cooling rate [19, 20]. Thus, it can be understood that the sample by sand cooling has a more obvious yield platform and a higher yield strength, while a lower tensile strength compared to the sample by air cooling, as shown in figure 1.

Figure 5. Simulated evolution of the carbon concentration field of an Fe-0.375 mol.% C alloy during cooling at 1.2°C/s for: (a) 20.7 s, 790.2°C; (b) 70.4 s, 730.5°C; (c) 137.4 s, 650.1°C; (d) 658.3 s, 25.0°C.

Figure 6. Simulated evolution of the carbon concentration field of an Fe-0.375 mol.% C alloy during cooling at 7°C/s for: (a) 3.5 s, 790.8°C; (b) 12.4 s, 728.0°C; (c) 30.4 s, 602.3°C; (d) 112.9 s, 25.0°C.
4.2. Effect of grain size

To investigate the influence of grain size on the carbon concentration field, simulations are performed for an Fe-0.375 mol.% C alloy with different α grain sizes after isothermal heating at 815°C for 300 s and then cooled at 1.2°C/s. The results are presented in figure 7. The simulation conditions of figure 7 (a) are identical with those used in figure 5. For the simulation of figure 7 (b), the number of initial α grains is set as 60, corresponding to the average α grain size of 9.7 μm. Other conditions are also identical with those used in figures 5 and 7 (a). As shown, the carbon concentration fields with different α grain sizes have the similar uniformity, indicating that the cooling process at 1.2°C/s provides sufficient time for carbon diffusion in both cases with different grain sizes. Thus, the α grain size has less influence on the formation of high concentration Cottrell atmospheres when cooled at 1.2°C/s. As discussed above, the yield platform is mainly affected by the carbon distribution and the formation of high concentration Cottrell atmospheres. Accordingly, it is understandable that the two samples with different α grain sizes have similar yield platform widths when cooled by sand cooling as shown in figure 2. On the other hand, it is well known that fine grain size will contribute to increasing both yield strength and tensile strength [3,4,21-26]. Thus, as shown in figure 2, the sample with the average α grain size of 6.9 μm exhibits both higher yield strength and tensile strength than that of the sample with the average α grain size of 9.7 μm.

![Figure 7](image_url)

**Figure 7.** Simulated carbon distribution of an Fe-0.375 mol.% C alloy after cooling to room temperature at 1.2°C/s with different average α grain sizes: (a) 6.9 μm; (b) 9.7 μm.

5. Conclusions

A two-dimensional cellular automaton model is applied to simulate the ferrite (α)-austenite (γ) transformation in a low-carbon steel during different heat treatment processes. The α→γ transformation during isothermal heating at 815°C and the γ→α transformation during continuous cooling at 1.2°C/s and 7°C/s are simulated. During the isothermal heating, the γ phase fraction increases evidently during the period of 0.1 s ~ 10 s. The mean carbon concentration in the α phase decreases with time while the mean carbon concentration in the γ phase increases to a maximum at the early stage of α→γ transformation and then decreases gradually, approaching the equilibrium value. After holding for 300 s, the carbon concentrations in both the α phase and γ phase reach their respective equilibrium values. The simulated microstructures agree well with the SEM images. After subsequent cooling to room temperature, the sample cooling at 1.2°C/s exhibits a uniform carbon distribution, while a non-uniform carbon concentration field is obtained when cooled at 7°C/s. The uniformities of the carbon concentration fields with different α grain sizes are similar in the case of cooling at 1.2°C/s. The simulation results are used to understand the experimental phenomena that the sample sand cooled exhibits a longer and more obvious yield platform than samples air cooled, while the samples with different grain sizes have similar yield platforms when cooled by sand cooling.
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