

Postprint: Simulation of Proeutectoid Ferrite Growth Kinetics Under a Mixed-Control Model Considering Dislocation Interactions

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Date: 2023-03-19T00:00:00+00:00

Abstract

An interface reaction-diffusion mixed control model that considers the interaction of dislocations accompanying steps was established and employed to simulate the growth processes of proeutectoid ferrite with two steps and multiple steps. The results indicate that when only two steps are present and their horizontal separation exceeds the critical distance, mutual attraction between the steps occurs, which can reduce the growth rate of the leading step to some extent; when the horizontal separation is less than the critical distance, the steps mutually repel, thereby increasing the growth rate of the leading step. Under multi-step conditions, the interaction among dislocations accompanying the steps modifies the step coalescence behavior and produces a certain effect on the step growth rate.

Full Text

Simulation of Growth Kinetics of Pro-Eutectoid Ferrite Using Mixed-Control Model with Consideration of Dislocation Interaction

Abstract

During austenite to ferrite transformation, the lattice structure transforms from fcc to bcc, resulting in a clearly distinguishable austenite and ferrite interface. The short-range diffusion of Fe and C atoms across the interface causes its movement, referred to as interface migration. On the other hand, the C rejected by the ferrite during the austenite to ferrite transformation in Fe-C alloys accumulates ahead of the moving interface. This pile-up of C atoms is dependent on the long-range diffusion of C in austenite and also influences the ferrite growth kinetics. Experimental observations indicate that dislocations are always migrating

with ledges during ledgewise growth. The local stress field of dislocations is considered to alter the solute concentration at the riser of ledges and causes a complex diffusion field interaction among ledges as they migrate. Some established works by other researchers have already taken this effect into consideration when studying phase transformation kinetics. However, these works were limited to diffusion-controlled cases and could hardly explain some experimental results. In this work, a ledgewise growth model considering migration of the austenite/ferrite interface, C diffusion in austenite, and especially elastic interactions between dislocations moving with ferrite ledges was established, and all the simulated results were qualitatively similar to reported experimental results. Calculated results showed that the C concentration at the riser of ledges was changed by the elastic stress of these dislocations, which would further change the growth behavior of ledges. In the growth behavior simulations of two ledges, the horizontal distance between the two ledges was found to play a key role in determining the growth kinetics. When the horizontal distance was larger than the critical distance, an attractive phenomenon between the two ledges was found to decelerate the leading step, while a repulsive phenomenon accelerated the leading ledge if the horizontal distance was smaller than this value. Compared with simulation results without considering elastic interactions between dislocations, in the growth behavior simulations of multi-ledge with elastic dislocation interactions, both the coalescence behavior of ledges and the growth rate of the leading step were changed.

Keywords: pro-eutectoid ferrite, mixed-control model, ledgewise growth kinetics

The pro-eutectoid ferrite growth process in steel involves two simultaneous processes: the long-range diffusion of solute C atoms from the interface into the parent austenite phase, and the crystal structure transformation from the parent austenite fcc structure to the new ferrite bcc structure at the interface. Consequently, two types of models have been developed for pro-eutectoid ferrite growth: diffusion-controlled models and interface-controlled models. Diffusion-controlled models, also known as local equilibrium models, assume that interface reactions occur very rapidly and that ferrite growth is controlled by C diffusion in austenite. Interface-controlled models, conversely, assume that C diffusion is very rapid during transformation and that ferrite growth depends on the rate of interface reactions. Diffusion-controlled models accurately describe ferrite growth kinetics at lower transformation temperatures and higher C contents, while interface reaction-controlled models show better agreement with experimental results when the C concentrations in parent austenite and new ferrite are similar. Based on these two models, researchers have proposed that pro-eutectoid ferrite growth is controlled by both interface reactions and C diffusion, i.e., an interface-diffusion mixed-control model.

In recent years, extensive computational work has been conducted on ferrite growth. Enomoto developed a diffusion-controlled two-dimensional ledge growth

model and investigated ferrite ledge growth processes. Hoyt pointed out that diffusion-controlled ledge models are not applicable to Fe-C alloys and argued that pro-eutectoid ferrite growth in Fe-C alloys is not completely controlled by C diffusion. Our research group introduced interface reaction factors based on diffusion-controlled ledge models and conducted preliminary studies on pro-eutectoid ferrite ledge growth. Results indicated that ferrite ledge growth rates are controlled by both C diffusion at the interface and interface reactions. When interface mobility is high, C diffusion from the two-phase interface into austenite becomes the dominant factor affecting ledge growth rate, while at low interface mobility, the interface reaction rate determines ledge growth speed.

Hirth found that ledges are often accompanied by dislocations during growth. Studies have shown that the stress field generated by these dislocations affects ferrite ledge growth. During ledge growth, dislocations accompanying ledges influence the stress field at the two-phase interface, thereby affecting ledge growth kinetics. Kamat and Hirth and Enomoto and Hirth explored the effects of dislocations on ledge growth, but did not consider interface reaction factors, and such simulations were only discussed for Al-Ag alloy transformations. Therefore, systematic investigation of dislocation-ledge interactions during ferrite ledge growth is necessary.

Building on our previous mixed-control ledge growth model, this work introduces interactions between dislocations accompanying ledges into the pro-eutectoid ferrite growth process in Fe-C alloys, investigates the effects of dislocations on ferrite ledge growth, and compares calculated results with experimental data.

1.1 Ledge Growth Mechanism

Based on our previous mixed-control ledge growth model, we assume that ferrite nucleates at austenite grain boundaries and grows into the surrounding austenite grains. As shown in [Figure 1: see original paper], the y-axis is along the grain boundary direction, and after nucleation at the austenite grain boundary, ledges grow along the x-axis into the austenite grain. Since the ledge terrace plane has a coherent or semi-coherent structure, ferrite growth in this direction is extremely slow and can be neglected, while the ledge riser has a disordered structure that can migrate stably. The migration rate of the ledge riser in this direction represents the ferrite growth rate. Additionally, the ledge riser remains planar during forward migration, meaning all points on the riser migrate at the same velocity.

Assuming each ledge is accompanied by one edge dislocation located at the junction between the previous ledge terrace plane and the current ledge riser, the dislocation moves with the ledge. During ledge motion, dislocations on other ledges interact with the dislocation on ledge i (Fig. 1), affecting the C atom concentration on the austenite side of ledge i 's riser and thereby influencing the growth rate of ledge i .

1.2 Mixed-Control Model Considering Dislocation Stress Field

The C diffusion process can be described using a two-dimensional diffusion equation:

$$\frac{\partial c}{\partial t} = D \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right)$$

where c is the C concentration in the parent phase, D is the diffusion coefficient of C in austenite, and t is time. The C diffusion flux at the ferrite/austenite interface consists of two components: one part is the flux of C atoms released during ferrite formation, $J_{\text{int}+\Delta}$, and the other part is the flux of C atoms diffusing into the parent austenite, J_x , as shown in [Figure 2: see original paper]. The diffusion flux can be expressed as:

$$J_{\text{int}+\Delta} = \frac{v_i(c_m - c_\alpha)}{h}$$

where c_m and c_α are the C concentrations on the austenite and ferrite sides of the interface without considering dislocation interactions, respectively, and v_i is the migration rate of ledge i 's riser. Since $J_{\text{int}+\Delta}$ and J_x are not equal, c_m continuously changes during transformation. In the early stage of ferrite nucleation, c_m gradually increases from the initial matrix concentration c_0 toward the equilibrium concentration. As the reaction proceeds, c_m approaches the equilibrium value.

Without considering the effect of dislocation interactions on ledge growth, the thermodynamic driving force is considered to drive riser migration, determined by the free energy difference between austenite at the interface and the matrix. Therefore, the force F acting on a unit length of ledge can be expressed as:

$$F = \frac{\Delta G_{\text{int}} V_m}{h}$$

where V_m is the molar volume of the ferrite precipitate and h is the ledge height. If the C concentration in the matrix is sufficiently small, the free energy change can be approximated as:

$$\Delta G_{\text{int}} \approx RT \ln \left(\frac{c_m}{c_0} \right)$$

where R is the ideal gas constant and Θ is the transformation temperature.

Considering dislocation interaction effects, the stress acting on the dislocation at ledge i due to the stress field of the dislocation at ledge j in Fig. 1 can be expressed as:

$$\sigma_{ij} = \frac{\mu b}{2\pi(1-\nu)} \Phi(x_i, y_i, x_j, y_j)$$

where μ and ν are the shear modulus and Poisson's ratio of the matrix, respectively, b is the magnitude of the Burgers vector of the dislocation on the ledge terrace, Φ is a function representing the magnitude of elastic stress, and (x_i, y_i) and (x_j, y_j) are the coordinates of ledges i and j , respectively. For multiple continuous ledges, the total elastic force F_{elastic} acting on a unit length of ledge i can be expressed as:

$$F_{\text{elastic}} = \sum_{j=s, j \neq i}^n \sigma_{ij}$$

where s and n are the indices of the starting and most recently formed ledges, respectively. After considering dislocation interactions, the equivalent thermodynamic force F'_{th} driving riser migration can be expressed as:

$$F'_{\text{th}} = F_{\text{th}} + F_{\text{elastic}}$$

The C concentration on the austenite side of the ledge after considering dislocation interactions, c'_m , can be determined by:

$$c'_m = c_m + \Delta c_m$$

To obtain the C concentration on the austenite side of the ledge front without dislocation effects, c_m , we consider only one-dimensional diffusion. Assuming no diffusion occurs in the y-direction at the ledge riser (i.e., only C diffusion from ferrite to austenite along the x-direction is considered at the interface), and combining with Eq. (2), Fick's second law gives:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

The growth rate of pro-eutectoid ferrite, i.e., the migration rate of ledge i 's riser, can be expressed as:

$$v_i = M \Delta G'_{\text{int}}$$

where M is the generalized interface mobility and $\Delta G'_{\text{int}}$ is the free energy difference driving interface migration. The $\Delta G'_{\text{int}}$ in Eq. (10) differs from that in Eq. (4). ΔG_{th} is a thermodynamically approximate free energy difference for conveniently considering dislocation interactions, while $\Delta G'_{\text{int}}$ represents the

portion of the total transformation driving force acting on interface reactions, obtained from experimental data. M can be calculated as:

$$M = M_0 \exp\left(-\frac{E}{RT}\right)$$

where the activation energy $E = 140$ kJ/mol and M_0 is a constant that varies with interface conditions, with experimental values ranging from 0.058 to 5000 mol·m/(J·s). In this work, $M_0 = 51.9$ mol·m/(J·s). $\Delta G'_{\text{int}}$ can be calculated as:

$$\Delta G'_{\text{int}} = \chi(c'_m - c_{\text{eq}})$$

where the proportionality constant $\chi = 110$ J/mol and c_{eq} is the equilibrium C concentration in austenite at the transformation temperature.

According to Enomoto and Hirth, the effect of dislocation interactions on the C concentration ahead of the ledge in austenite can be explained thermodynamically. [Figure 3: see original paper] shows a schematic of the free energy change caused by C concentration variation in austenite ahead of the two-phase interface when dislocation interactions are considered. Here, c'_m is the C concentration in austenite ahead of the interface obtained when the force from dislocations on the ledge, F_{elastic} , is negative. The free energy change caused by F_{elastic} is denoted as $\Delta G_{\text{elastic}}$. When $\Delta G_{\text{th}} > 0$, transformation proceeds, and the total free energy change after adding $\Delta G_{\text{elastic}}$ is positive. For ledge i , considering dislocation interactions gives $\Delta G'_{\text{th}} = \Delta G_{\text{th}} + \Delta G_{\text{elastic}}$. From Fig. 3a, if $\Delta G_{\text{elastic}} > 0$, then c'_m can be obtained from Eq. (8). When $\Delta G_{\text{elastic}} < 0$, the schematic of free energy change caused by C concentration ahead of the interface can be described by Fig. 3b.

1.3 Simulation Method

The finite difference method was employed to simulate ledge growth of proeutectoid ferrite at austenite grain boundaries, comprehensively considering C diffusion from the interface into austenite, interface reactions, and the stress field of dislocations accompanying ledges. To ensure ledge shape remains unchanged during motion, all points on the same ledge riser move forward at the same velocity. The coordinate system was fixed at the ferrite nucleation site (the original austenite grain boundary), and at each simulation step, the effect of the stress field from dislocations on the C concentration on the austenite side of ledges was considered.

For convenient finite difference calculations, dimensionless variables were defined for concentration c , time t , growth rate v_i , and coordinates x, y :

$$U = \frac{c - c_0}{c_{\text{eq}} - c_0}, \quad T = \frac{Dt}{h^2}, \quad V = \frac{vh}{D}, \quad X = \frac{x}{h}, \quad Y = \frac{y}{h}$$

The initial condition corresponds to a uniform C distribution in the austenite structure at a specific temperature. As ferrite precipitates, at time step $T = k$, the current migration rate of the ledge riser V_k can be calculated from Eqs. (10)-(12), the C concentration on the austenite side of the interface U_k from Eq. (9), and the C concentration on the austenite side of the ledge interface after considering dislocation interactions U'_k from Eqs. (3)-(8). Then, from Eq. (1), the C concentration at every grid point in the entire region U_{k+1} can be obtained. The next calculation step, $T = k + 1$, then proceeds by repeating the process for step $T = k$.

2. Results and Discussion

For convenient comparison with our previous results, simulations of proeutectoid ferrite growth kinetics were performed for an Fe-0.34%C (atomic fraction) alloy undergoing isothermal transformation at 720 °C. Using the TCFE7 database in Thermo-Calc, the equilibrium concentrations at this temperature were calculated as $c_{\text{eq}} = 3.67\%$ and $c_{\alpha} = 0.092\%$. The C diffusion coefficient in austenite at this temperature, obtained from the MOB2 database in Dictra, was $D = 4.398 \times 10^{-13} \text{ m}^2/\text{s}$. The ferrite ledge height was $h = 0.066 \text{ mm}$, the Burgers vector b of the dislocation was along the close-packed direction of ferrite with $b = \frac{1}{2}a$, the ferrite lattice constant $a = 0.28664 \text{ nm}$, and the matrix Poisson's ratio and shear modulus were $\nu = 0.28$ and $\mu = 83 \text{ GPa}$, respectively. For simplicity, only the ferrite growth stage was simulated, neglecting the nucleation stage, which was assumed to require negligible time. Additionally, the parent austenite grain was assumed to be much larger than the new ferrite grain, with uniform nucleation occurring at fixed time intervals to form each ferrite ledge.

2.1 Growth Process of Two Ferrite Ledges

To investigate the effect of the dislocation stress field on the C concentration on the austenite side of ledge risers, the growth process of a ferrite lamella containing only two ledges was considered.

[Figure 4: see original paper]a shows F_{elastic} plotted according to Eq. (6), where $X_d = X_1 - X_2$, with X_1 , X_2 , and X_d representing the dimensionless horizontal coordinates of ledge 1, ledge 2, and the horizontal distance between the two ledges, respectively. Since ledge height is constant, only the effect of horizontal distance X needs to be considered. When each ledge contains one dislocation, the force F_{elastic} acting on ledge 1 (the leading ledge) due to dislocation interactions is initially negative, indicating mutual attraction between the two ledges. At $X_d \approx 2.3$, the value approaches zero. When $X_d \approx 1.0$, the sign changes—this distance is defined as the critical distance. Beyond this point, as X_d increases further, the two ledges repel each other, with the repulsive effect reaching a maximum at a certain X_d value before gradually weakening and eventually stabilizing. The effect of dislocation interactions on ledge 2 is opposite to that on ledge 1.

[Figure 4: see original paper]b shows the change in C concentration on the austenite side of ledge 1, Δc_m , caused by dislocation interactions. The figure reveals that Δc_m has a strong relationship with X_d and also depends significantly on c_m . As c_m increases, Δc_m gradually decreases, while the opposite occurs for c'_m . The variation range of Δc_m is smallest when $c_m = c_{eq}$. The effect of X_d on Δc_m follows the same trend as its effect on $F_{elastic}$. When the two ledges attract each other, c'_m decreases, causing ledge 1's growth rate to increase and ledge 2's growth rate to decrease. When they repel each other, c'_m increases, causing ledge 1's growth rate to decrease and ledge 2's growth rate to increase.

To investigate the different effects of dislocation interactions on ledge growth at different stages, two different total dimensionless simulation times were employed: $T_1 = 6.25 \times 10^{-2}$ and $T_2 = 6.25 \times 10^{-1}$. Ledge 2 formed and began growing at times $T_1/2$ and $T_2/2$, respectively.

[Figure 5: see original paper] shows the simulated ferrite growth morphologies for a total transformation time of $T_1 = 6.25 \times 10^{-2}$, both with and without dislocation interactions. For improved accuracy, the step sizes for horizontal coordinate X and vertical coordinate Y in the simulation were both $DX = DY = 1/4$. The coordinates shown in Fig. 5 are expanded by a factor of 4. The results demonstrate that dislocation interactions between ledges severely restrict the growth of ledge 2. Due to its slow growth, diffusion is sufficient, resulting in an almost zero C concentration gradient around ledge 2 (Fig. 5a). For ledge 1, however, when dislocation interactions are considered, the ledge length is greater during the simulated time period, though the difference is not significant. Additionally, the C concentration gradient around ledge 1 in this case (Fig. 5a) is larger than when dislocation interactions are neglected, resulting in a higher lateral migration rate and thus greater growth rate for ledge 1.

[Figure 6: see original paper] shows the evolution of the dimensionless C concentration U on the austenite side and the dimensionless migration rate V of the ledge risers for the two cases. Without dislocation interactions, ledge 1 initially has $U = 0$ ($c_m = c_0$). As the ledge grows, U rapidly increases while V rapidly decreases, eventually reaching stable values after a short time, after which ledge 1 enters a steady growth stage. The appearance of ledge 2 has no effect on ledge 1's growth rate, and ledge 2 reaches a stable growth state similar to ledge 1 (Fig. 6a). In contrast, when dislocation interactions are considered, the appearance of ledge 2 causes a slight decrease in U for ledge 1 (Fig. 6b). Combined with Fig. 5, where the distance between the two ledges $X_d < 1$, the two ledges repel each other due to dislocation interactions, increasing ledge 1's growth rate. The steady growth state is no longer maintained. As growth continues, since ledge 1's growth rate exceeds that of ledge 2, their distance continuously increases, gradually weakening the repulsive effect. Under the combined influence of dislocation interactions, C diffusion, and interface reactions, ledge 1's growth rate gradually decreases while ledge 2's growth rate gradually increases, reducing the rate difference between them, though this process occurs relatively slowly.

[Figure 7: see original paper] shows the ferrite growth morphologies for a total simulation time of $T_2 = 6.25 \times 10^{-1}$, both with and without dislocation interactions. At time T_2 , when dislocation interactions are considered, ledge 1 is shorter and its diffusion field extends further ahead of the interface (Fig. 7a) because its growth rate V is smaller, allowing more time for C diffusion. The opposite is observed for ledge 2 (Fig. 7b).

[Figure 8: see original paper] shows the evolution of U and V for the two ledges in both cases. The behavior without dislocation interactions is similar to that observed for simulation time T_1 . However, when dislocation interactions are considered, at the moment ledge 2 forms, the distance between the two ledges is large, exceeding the critical distance, resulting in mutual attraction. This decreases V for ledge 1 (Fig. 8b). Under the influence of dislocation interactions, ledge 2 does not rapidly accumulate large amounts of C atoms ahead of its interface (Fig. 8a), allowing it to maintain high growth velocity for some time. As X_d gradually decreases and falls below the critical distance, the two ledges become mutually repulsive, making ledge 1's rate higher than ledge 2's. X_d then increases until it exceeds the critical distance again. This reciprocating process can be viewed as a "buffering process" (Fig. 8b), resulting from the combined effects of dislocation interactions, long-range C diffusion, and interface reactions. Subsequently, since the U values ahead of both ledges approach the equilibrium C content in austenite (dimensionless value of 1), the influence of dislocation interactions is greatly weakened, and the changes in growth rates V of ledges 1 and 2 gradually slow down, with their rate difference decreasing.

2.2 Growth Process of Multiple Ferrite Ledges

According to literature summarizing ledge growth simulation results, in cases with multiple ledges, smaller initial ledge spacing facilitates coalescence to form larger ledges, while larger initial spacing typically results in higher growth rates for leading ledges, making coalescence less likely. To examine the effect of dislocation interactions on ledge coalescence, a larger $M_0 = 51.9 \text{ mol} \cdot \text{m}/(\text{J} \cdot \text{s})$ and longer nucleation intervals were used to achieve larger initial ledge spacing. The simulation employed 10 total ledges with total time $T_2 = 6.25 \times 10^{-1}$, forming one ledge every $T_2/10$. The ferrite morphology at time T_2 is shown in [Figure 9: see original paper].

[Figure 9: see original paper]b shows the growth morphology without dislocation interactions, where no coalescence occurs among the 10 ledges. However, when dislocation interactions are considered (Fig. 9a), coalescence occurs and the morphology changes. Without dislocations, after reaching steady growth, the growth rate remains constant, and since the leading ledge has a higher velocity, no coalescence occurs. After reaching steady growth, the ledges no longer influence each other (Fig. 9b). With dislocation interactions, dislocations accompanying ledges 2, 3, ..., 10 all affect ledge 1's growth, resulting in shorter growth length for ledge 1 during time T compared to the case without dislo-

cation interactions. Additionally, under the mutual interaction of dislocations on adjacent ledges, some ledges coalesce—for example, ledges 4, 5, and 6 merge into one ledge, and ledges 8 and 9 merge into one ledge, with the merged ledges growing forward as a single large ledge (Fig. 9a).

In cases without dislocation interactions, both purely diffusion-controlled and interface-diffusion-controlled ledge models show that ledge growth rates reach stability within a short time, after which the leading ledge growth rate remains unchanged. Even if the leading ledge coalesces with others, the merged ledge continues to grow at the leading ledge's rate.

2.3 An Explanation for Nonlinear Growth of Ferrite Ledges

Eichen et al. measured pro-eutectoid ferrite growth curves in Fe-0.305%C alloy isothermally transformed at 740 °C using thermionic emission microscopy. Experimental results showed that ledge 1 length did not increase linearly but exhibited irregular behavior. For instance, after approximately linear growth for some time, the growth rate showed noticeable fluctuations before gradually returning to approximately linear growth ([Figure 10: see original paper]b). According to our simulation results under these conditions ($M_0 = 0.27 \text{ mol} \cdot \text{m}/(\text{J} \cdot \text{s})$), this growth behavior may result from the appearance of new ledges and the influence of interactions between dislocations accompanying the ledges on the growth process. When a second ledge is introduced at the moment when the leading ledge's linear growth begins to change, the large distance between the two ledges causes mutual attraction, decreasing ledge 1's growth rate v_1 . This is followed by a “buffering process” where v_1 decreases to a minimum, then gradually increases, decreases again, and finally stabilizes (Fig. 10a). The linear increase in ledge 1 length L_1 with time is disrupted by the appearance of the second ledge, and after some time, approximate linear growth resumes (Fig. 10b). The simulation results satisfactorily describe the experimentally observed behavior, indicating that the mixed-control model considering interactions between dislocations accompanying ledges can appropriately describe this phenomenon. As the number of ledges increases, dislocation interactions become more complex, causing the curve of pro-eutectoid ferrite ledge length versus time to deviate further from linear growth. Similar phenomena were observed in experimental measurements of pro-eutectoid ferrite ledge growth rates by Kinsman et al. and Simonen et al.

Conclusions

1. Based on the mixed-control ledge growth model, a model for simulating pro-eutectoid ferrite growth was established by considering elastic interactions between dislocations accompanying ledges.
2. In the case of only two ferrite ledges, dislocation interactions depend on the horizontal spacing between ledges. When the horizontal spacing is smaller than the critical distance, the two ledges exhibit repulsive interaction,

which increases the growth rate of the leading ledge (ledge 1) and decreases that of the trailing ledge (ledge 2). This differs from the case without dislocation interactions where ledge growth rates remain unchanged once steady growth is reached. If the horizontal spacing exceeds the critical distance, the interaction becomes attractive, producing effects opposite to those described above.

3. In cases with multiple ledges, dislocation interactions alter ledge growth behavior and affect growth kinetics. The mixed-control model considering interactions between dislocations accompanying ledges can reasonably explain experimental observations that leading pro-eutectoid ferrite ledges do not grow strictly linearly.

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