Cellular automaton modelling of M₇C₃ carbide growth during solidification of Fe-C-Cr alloy

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Abstract. A microscopic cellular automaton combined with macroscopic heat and solute transport was developed to simulate the mutual growth and evolution of austenite and M₇C₃ carbide grains during Fe-C-Cr ternary alloy solidification process. The diffusion of solute C and Cr are contributed together to the constitutional undercooling, together with curvature undercooling, for obtaining the grain growth rate of austenite and M₇C₃ carbide. Results show that, the absorption of solute C and Cr by M₇C₃ grain and rejection by austenite grain promote the two grains' cooperative growth. Once they approach to each other, the austenite grain quickly overgrows towards the M₇C₃ grain till finally envelops it. The simulated solidification morphology of the Fe-4wt%C-17wt%Cr alloy, predicted averaged grain size of M₇C₃ carbides and C and Cr concentration in austenite grains agree with the experimental measurements and solidification path prediction. The predicted average liquid concentration curve fits with the LR, GS and PE prediction at the initial M₇C₃ precipitation regime and after austenite grains fully enveloping towards the M₇C₃ grains, returns to overlap the LR, GS and PE prediction curves.

1. Introduction

Fe-C-Cr based alloys have been widely applied in metallurgical, mineral and mechanical fields due to their great wear resistance [1], in which the carbides, especially M₇C₃ carbide's amount, size, morphology and distribution in the microstructure contribute much to the final properties. As reported, the coarse M₇C₃ carbide precipitated in Fe-C-Cr melt spoils the continuity of the matrix, speeds up the formation and extension of the crack and consequently shortens the operation span of the alloys [2].

The theoretical and experimental researches have shown that M₇C₃ carbide grows in a faceted hexagonal close-packed (HCP) structure, which behaviours as an irregular hexagonal shape in 2D section [3]. The austenite grows in a dendritic structure when growing isolatively. With solidification proceeding, the precipitated austenite and M₇C₃ carbide grains grow up mutually, while the growing details are not very clear. Besides the theoretical and experimental studies, the numerical simulation gives great help in revealing the solidification mechanics. And among the field, the microscopic cellular automaton has gained great favour [4] in quantitatively evaluating the interaction between concentration evolution and grain growth, combining with macroscopic melt flow, heat and solute transport, and describing the detailed dendritic structure with an actual calculation size and economic calculation cost.

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Thus the present paper studied the mutual growth of M$_7$C$_3$ carbide and austenite grains during solidification of a Fe-4wt%C-17wt%Cr ternary alloy with microscopic cellular automaton model. The study is expected to clarify their mutual growth mechanics and further control the distribution of M$_7$C$_3$ carbide grains in austenite matrix for obtaining better mechanical properties of the alloy.

2. Cellular automaton model

2.1. Assumptions
A) The heat diffusion of the molten alloy and the release of the latent heat during the solidification are ignored. B) The melt flow is omitted. C) The interface is always kept as thermodynamic equilibrium with ignoring the thermodynamic undercooling and kinetic undercooling. D) The physical properties of the alloys are kept constant.

2.2. Temperature field
The temperature of the melt is uniformly cooled down with a constant cooling rate $\dot{T}$,

$$\frac{\partial T}{\partial t} = \dot{T}$$

(1)

Then it is updated through the explicit scheme.

2.3. Concentration field
The diffusion of solute $i$ (C or Cr) is governed by the following equation with zero flux condition at the region boundary,

$$\frac{\partial \bar{C}_i}{\partial t} = D \left( \frac{\partial^2 P}{\partial \bar{x}^2} \right) + D \left( \frac{\partial^2 P}{\partial \bar{y}^2} \right)$$

(2)

where $\bar{C}_i$ is the average solute concentration of solute $i$, expressed as $\bar{C}_i = f_y C_{\gamma,i} + f_mC_{M,i} + f_L C_{L,i}$. $f_y$, $f_M$ and $f_L$ are the mass fraction of austenite, M$_7$C$_3$ carbide and liquid; $C_{\gamma,i}$, $C_{M,i}$ and $C_{L,i}$ are the concentration of solute $i$ in austenite, M$_7$C$_3$ carbide and liquid, respectively.

$P_i$ is defined as an equivalent liquid concentration to unify the discontinuous solute concentration in phase and at interface, which is expressed as $C_i = f_y C_{\gamma,i} + \sum_n \Delta f_M^i C_{M,i}^n + f_L C_{L,i} / k_{p_y/L,i}$ at interface, $C_{L,i}$ in liquid, $\sum_n \Delta f_M^i C_{M,i}^n$ in carbide M and $C_{\gamma,i} / k_{p_y/L,i}$ in austenite cell, respectively. Here $\Delta f_M^i$ is the increase of M$_7$C$_3$ phase fraction at time step $n$, $C_{L,i}^n$ is the liquid concentration before M$_7$C$_3$ carbide's new formation at step $n$. $k_{p_y/L,i}$ is partition coefficient of solute $i$ at austenite/liquid interface, valued as 0.407 for C and 0.576 for Cr through solidification path prediction with partial equilibrium approximation [5, 6] and TCFE6 steel database [7].

The diffusion coefficient $D$ is expressed as $D = 0.5 [f_y D_{\gamma,i} + f_M D_{M,i} + f_L D_{L,i}] j + 0.5 [f_y D_{\gamma,i} + f_M D_{M,i} + f_L D_{L,i}] j + 1$. $D_{\gamma,i}$, $D_{M,i}$ and $D_{L,i}$ are the diffusion coefficient of solute $i$ in austenite, M$_7$C$_3$ carbide and liquid, valued as $D_{\gamma,C}$=2.57x10$^{-10}$ m$^2$/s, $D_{\gamma,CR}$=3.67x10$^{-14}$ m$^2$/s, $D_{M,C}$=D$_{M,CR}$=0, $D_{L,C}$=9.6x10$^{-10}$ m$^2$/s, $D_{L,CR}$=8.23x10$^{-10}$ m$^2$/s through retrieving from MOB2 steel mobility database [8].

2.4. Solidification path and nucleation
Upon the nominal concentration of Fe-4wt%C-17wt%Cr ternary alloy, the precipitation temperatures of austenite and M$_7$C$_3$ carbide are $T_\gamma$=1266 °C and $T_M$=1304 °C through solidification path prediction with partial equilibrium approximation.

The nucleation sites of M$_7$C$_3$ and austenite grains are initialized according to the experimental morphology [3]. At each phase’s nucleation site, the nucleation undercooling is randomly chosen among those nucleation undercoolings at the prescribed nucleation sites for the phase, which is set based on the idea of reference [9]. That is, the number of the nucleation sites, $N_n^{nucl}$, among the total volume $V$ is determined by $(n_{max}Vdn)$ at a certain nucleation undercooling, $\Delta T^{nucl}_n$, sequently chosen within the
given range, here is \( 0 - 20 \text{K} \). \( dn \) is the increase of grain density by the increase of undercooling \( d(\Delta T) \) as indicated in Gaussian distribution, \( dn/d(\Delta T) \), which is dependent of three parameters: the maximum nucleation density, \( n_{\text{max}} \), the maximum nucleation undercooking, \( \Delta T_{\text{max}} \), and its deviation, \( \Delta T_{\sigma} \). The data for \( M_7C_3 \) and austenite are \( n_{\text{max}} = 2 \times 10^6/\text{m}^3 \), \( \Delta T_{\text{max}} = 0.4 \text{K} \), \( \Delta T_{\sigma} = 0.1 \text{K} \) and \( n_{\text{max},Y} = 2 \times 10^6/\text{m}^3 \), \( \Delta T_{\text{max},Y} = 0.2 \text{K} \), \( \Delta T_{\sigma,Y} = 0.1 \text{K} \), respectively. These nucleation sites are randomly positioned in region \( V \) with the same \( \Delta T_{\nu} \). Through this way each phase is provided with a set of precribed nucleation undercoolings at its nucleation sites.

Once the local undercooling of the chosen nucleation site is larger than the prescribed nucleation undercooling of a certain phase, it nucleates. The state of the cell then changes to interface, and a random crystal orientation is given to the nucleation site. As for a nucleated austenite site, a random orientation ranged within \([-\pi/4, \pi/4]\) is given since it is growing in a four-fold symmetrical dendrite shape. Similarly, the random crystal orientation for a \( M_7C_3 \) carbide nucleus is ranged at \([-\pi/6+2, \pi/6+2]\) due to its six-fold symmetrical faceted hexagonal shape in 2D cross section, here +2 is just to distinguish its orientation with that of the austenite.

### 2.5. Interface equilibrium concentration

The total undercooling at the grain interface is the contribution of constitutional and curvature undercooling when omitting the thermodynamic and kinetic effects,

\[
T = T_L - \Delta T_R - \Delta T_C
\]

(3)

where \( T_L \) is liquidus temperature. The curvature undercooling \( \Delta T_R \) is expressed as

\[
\Delta T_R = \Gamma K f (\varphi, \theta)
\]

(4)

where the Gibbs-Thomson coefficient \( \Gamma \) is valued as \( 3.7 \times 10^{-7} \text{m-K} \) for austenite/liquid interface and \( 1.9 \times 10^{-7} \text{m-K} \) for \( M_7C_3 \) carbide/liquid interface [10]; interface curvature \( K \) is expressed through counting - cell technique [11] of the solid fractions around; \( f(\varphi, \theta) \) is an expression describing the anisotropy of the interface energy according to Gibbs-Thomson equation [12], \( f(\varphi, \theta) = 1 + (1 - k^2)\cos [k(\varphi - \theta)] \). The crystal symmetry parameter \( k \) is valued as 4 for FCC and 6 for HCP structure [13]; the anisotropy coefficient \( \epsilon \) is chosen as 0.04 for austenite and 0.025 for \( M_7C_3 \) carbide; \( \theta \) is crystallographic orientation; \( \varphi \) is the angle between the normal of the interface and x-axis, \( \varphi = \cos^{-1}[(\partial f_s/ \partial x)/ \sqrt{(\partial f_s/ \partial x)^2 + (\partial f_s/ \partial y)^2}] \).

The constitutional undercooling, \( \Delta T_C \), in a Fe-C-Cr alloy is the contribution of solute C and Cr,

\[
\Delta T_C = m_{L,C} (C_{0,C} - C_{L,C}^*) + m_{L,\text{Cr}} (C_{0,\text{Cr}} - C_{L,\text{Cr}}^*)
\]

(5)

where \( m_{L,i} \) is the liquidus slope of solute \( i \), its value is retrieved from solidification path prediction with partial equilibrium approximation for Fe-4wt%C-17wt%Cr alloy. They are \( m_{L,C} = -95.49 \text{K/\%wt} \) and \( m_{L,\text{Cr}} = 6.14 \text{K/\%wt} \) at austenite-liquid regime and \( m_{L,M,C} = 90.37 \text{K/\%wt} \) and \( m_{L,M,\text{Cr}} = 15.29 \text{K/\%wt} \) at \( M_7C_3 \) carbide-liquid regime. \( C_{L,i}^* \) is interface equilibrium concentration, expressed as \( C_{L,Y,i}^* \) for austenite and \( C_{L,M,i}^* \) for \( M_7C_3 \) carbide. \( C_{0,i} \) is initial concentration.

The intrinsic relation of the two solutes' diffusion for one unique interface growth rate is obtained from the definition of solute supersaturation [14]. In pure diffusion process, it is expressed as an Ivantsov function of Peclet number \( Pe_i \),

\[
\Omega = (C_{L,i}^* - C_{0,i})/(C_{L,Y,i}^* - C_{S,i}^*) = I_0(Pe_i) = Pe_i \exp(Pe_i) E_1(Pe_i)
\]

(6)

and \( C_{L,i}^* \) can be written for austenite \( (k_{p,Y/L,i}=\text{const}) \) and carbide interface \( (C_{M,i}=\text{const}) \) as

\[
C_{L,i}^* = \frac{C_{0,i}}{1 - (1 - k_{p,Y/L,i}) \Omega} \quad \text{and} \quad C_{L,i}^* = \frac{C_{0,i} - \Omega C_{M,i}^*}{1 - \Omega}
\]

(7)

where \( E_1(Pe_i) \) is the exponential integral function, \( E_1(Pe_i) = \int_{Pe_i}^{\infty} \exp(-\tau) / \tau d\tau \). Peclet number \( Pe_i \) is defined as
\[
Pc = \frac{V_n R}{2D_{li}} \tag{8}
\]
and the solute C and solute Cr's Peclet number has the relation of
\[
Pc = Pe_{cr} D_{li} / D_{li,C} \tag{9}
\]

Thus the constitutional undercooling \(\Delta T_C\) (equation (5)) can be expressed as an unique function of \(Pe_{cr}\), i.e. \(\Delta T_C = f(Pe_{cr})\). Substituting \(\Delta T_C\) (equation (5)) and \(\Delta T_R\) (equation (4)) into equation (3), the unknown \(Pe_{cr}\) can be obtained. Then the interface equilibrium concentration \(C_{li}^*\) is got from equation (7).

2.6. Interface growth rate and solid fraction

The interface growth rate, \(\bar{V}_n\), is calculated through the solute conservation at solid/liquid interface,
\[
\bar{V}_n(C_{li}^* - C_{s,i}) = \left[-D_{li} \left( \frac{\partial C_{s,i}}{\partial x} + \frac{\partial C_{l,i}}{\partial y} \right) + D_{s,i} \left( \frac{\partial C_{s,i}}{\partial x} + \frac{\partial C_{s,i}}{\partial y} \right) \right] \cdot \bar{n} \tag{10}
\]
Then the solid fraction is updated,
\[
f_S^{n+1} = f_S^n + \Delta f_S \tag{11}
\]
where
\[
\Delta f_S = \frac{V_i \Delta t \Delta s + V_j \Delta t \Delta s - V_i V_j \Delta t^2}{\Delta s^2} = \frac{\Delta t}{\Delta s} \left[ V_x + V_y - V_x \frac{\Delta t}{\Delta x} \right] \tag{12}
\]
Upon the austenite growth, a disturbance function, \(1 + A(1 - 2\text{Rand}())\), is multiplied with \(\Delta f_S\) to describe the influence of interfacial disturbance on dendrite growth, where \(A\) is chosen as 0.1; \(\text{Rand}()\) is a random number within [0,1]. As for \(\text{M}_{\text{C}_3}\) carbide, a shape factor \(G\) is adopted to eliminate the mesh anisotropy, which is related to the state of the nearest, second, third and fourth order adjacent neighbour group, \(S_{i}^{I}, S_{i}^{II}, S_{i}^{III}\) and \(S_{i}^{IV}\).
\[
G = \min \left[ 1, \frac{1}{4} \left( \frac{\sum_{m=1}^{4} S_{m}^{I} + \frac{1}{\sqrt{2}} \sum_{m=1}^{4} S_{m}^{II} + \frac{1}{\sqrt{2}} \sum_{m=1}^{4} S_{m}^{III} + \frac{1}{\sqrt{2}} \sum_{m=1}^{4} S_{m}^{IV} \right) \right], \quad S_m = \begin{cases} 0 & (f_{s,m} < 1) \\ 1 & (f_{s,m} = 1) \end{cases} \tag{13}
\]

2.7. Solid concentration

An austenite cell's concentration is updated through the accumulation of the newly solidified solutes to the existing ones,
\[
C_{s,i} (C_{s,i} + k_{p,i} C_{li}^{n-1} \Delta f_S) / (f_S^n + \Delta f_S) \tag{14}
\]
The \(\text{M}_{\text{C}_3}\) cell's concentration is set fixed.

2.8. Solute redistribution

With the grain growth, the solutes are apt to be absorbed from or rejected to the liquid interface due to their solubility in solids. The lacked or accumulated concentration at the liquid interface needs to be evened up, that is, solute redistribution.

2.8.1. Neighbourhood relations. According to the crystal morphologies, a Moore relation is adopted for austenite grain, and a hexagonal-like neighbourhood relation [15] is adopted for \(\text{M}_{\text{C}_3}\) grain.

2.8.2. Solute redistribution for \(\text{M}_{\text{C}_3}\) carbide. With \(\text{M}_{\text{C}_3}\) phase fraction increasing and the high solubility of C and Cr in \(\text{M}_{\text{C}_3}\) phase, i.e. the local partition coefficients \(k_{p,M/Li} > 1\), the solutes keep be absorbed from the liquid interface and spread over the neighbour cells. Assuming \(C_{li}^{n}\) and \(C_{li}^{n-1}\) are the concentration of solute i and phase fraction of \(\text{M}_{\text{C}_3}\) and liquid for the present cell at moment n. Once there is an increase \(\Delta f_m\) of \(\text{M}_{\text{C}_3}\) at n+1 moment, the composition of the residual liquid updates accordingly:
(1) If \( \Delta f_\text{M} < f_\text{L}^n \), the interface cell absorbs the solute from its residual liquid, then its liquid concentration decreases to \( C_{L,M,i}^{n+1} = (C_{L,M,i}^n - \Delta f_\text{M} C_{M,i})/(f_\text{L}^n - \Delta f_\text{M}) \).

If \( C_{L,M,i}^{n+1} < 0 \), the lacked concentration, \( \Delta C_i = C_{L,M,i}^{n+1}(f_\text{L}^n - \Delta f_\text{M}) \), will be compensated evenly by the available neighbour cells which have remaining liquid, then \( C_{L,M,i}^{n+1} = 0 \); if \( C_{L,M,i}^{n+1} > C_{L,M,i}^* \), the excess solute \( \Delta C_i = (C_{L,M,i}^* - C_{L,M,i}^n)(f_\text{L}^n - \Delta f_\text{M}) \) will be re-distributed evenly to the available neighbour cells containing liquid, then set \( C_{L,M,i}^{n+1} = C_{L,M,i}^* \).

(2) If \( \Delta f_\text{M} \geq f_\text{L}^n \), setting \( \Delta f_\text{M} = f_\text{L}^n \). The cell changes its state to M-C3 solid. The solid concentration is set \( C_{M,i} = \text{const.} \) The absorbed solute \( \Delta C_i = (C_{M,i} - C_{L,M,i}^n) \Delta f_\text{M} \) is provided evenly by the available neighbour cells. Then set \( C_{L,M,i}^{n+1} = 0 \).

2.8.3. Solute redistribution for austenite. The solute redistribution around austenite grain is opposite to that around M-C3 carbide since \( k_{\text{P},\text{Y}/\text{L},i} < 1 \). With the growth of austenite grains, the C and Cr solutes are rejected from the austenite and accumulated in the residual liquid at the interface, which need to be redistributed around. The solute redistribution for austenite follows the similar routine as those for M-C3.

2.9. Determination of time step

\[
\Delta t \leq 0.2 \min(\Delta x^2/D_{L,C}, \Delta x^2/D_{L,C_3}, \Delta x/V_{\text{max}}, \Delta t_0)
\]

where \( D_{L,i} \) is the diffusion coefficient of solute \( i \) in liquid, \( \Delta t_0 \) is the initial time step.

2.10. Solution

A) Setting the initial concentration \( C_{0,i} \) and the initial temperature for the total region. B) Determining the time step (equation (15)). C) Cooling down the melt uniformly with a constant cooling rate (equation (1)). D) Once the temperature of a certain cell approaches the nucleation undercooling of M-C3 or austenite, the cell is nucleated and labelled as an interface one. E) Obtaining the unique Peclet number of solute Cr through coupling the expressions of the local undercooling (equation (3)), curvature undercooling (equation (4)), constitutional undercooling (equation (5)) and interface equilibrium concentration (equation (6)) with each solute Peclet number \( P_{\text{e},i} \) (equation (8)). F) Obtaining the interface equilibrium concentration of solute Cr, i.e. \( C_{L,Cr}^* \), through equation (7). G) Updating the grain growth rate and the solid fraction through equation (10) and equation (11). H) Repeating steps E) - G) for iteration until the interface curvature is converged. I) Updating the solid concentration through equation (14). J) Redistributing solute concentration through section 2.8. K) Solving the concentration field (equation (2)). L) Going back to step B) until the calculation region is completely solidified.

3. Solidification microstructure evolution of Fe-4wt%C-17wt%Cr alloy

According to the experimental cooling condition and obtained microstructure morphology of Fe-4wt%C-17wt%Cr alloy [3], a 700 \( \mu \text{m} \times 520 \mu \text{m} \) 2D region with CA mesh size 2 \( \mu \text{m} \times 2 \mu \text{m} \) is adopted. The initial undercooling of the melt is set as \( -4 \text{ K} \) from the liquidus temperature 1304 °C and the constant cooling rate \( \dot{T} \) is chosen as -1.3 K/s corresponding to the graphite mould cooling condition. The austenite and M-C3 carbide nucleation sites were set according to the microstructure morphology [3]. The nucleation undercooling was set randomly.

The mutual growth of M-C3 grain and adjacent austenite grains during solidification can be seen from austenite phase fraction evolution in figure 1. The envelope of a single austenite grain B to a M-C3 grain A can be found at the bottom centre of the region. The M-C3 grain A keeps absorbing solutes while the adjacent austenite grains B keep rejecting them as they grow up. Once the two kinds of grains grow up to approach each other, the mutual complement of the solutes at the interface accelerate their growth till finally the austenite grains B totally envelope the M-C3 grain A.
Figure 1. Enveloping of austenite grains to M$_7$C$_3$ grain A and F during solidification: (a) t=27.00 s (b) t=27.26 s (c) t=27.53 s and (d) t=27.88 s.

Figure 2. Concentration of solute (a) C and (b) Cr around M$_7$C$_3$ grain A and austenite grain B during enveloping.

Figure 3. Concentration distribution of solute (a) C and (b) Cr around a separated M$_7$C$_3$ grain C and (c) C and (d) Cr around austenite grain D as labelled in figure 1.

Figure 4. Final solidification microstructure (a) simulated and (b) experimental [3] and simulated solute concentration of (c) C and (d) Cr for Fe-4wt%C-17wt%Cr alloy.

Figure 5. Predicted average liquid composition of Cr with respect to that of C for Fe-4wt%C-17wt%Cr alloy by the present model, comparing with the solidification path prediction by LR, GS and PE approximations. The thin grey curves delimit the domains of the liquidus surfaces of different phases in the system.
Figure 2 shows the solute concentration evolution along the horizontal centerline of austenite grain B and M-C3 grain A during this envelope. Due to the partition of solutes, the lacked solute concentration is over double of the liquid concentration at M7C3/liquid interface, while the accumulated concentration at austenite grain interface is merely one half of its interface liquid concentration. As seen, at 27.00 s, the liquid concentration at the right-side interface of grain A, i.e. in between grain A and B, which is 1.6wt%C and 7.4wt%Cr, is lower than the left-side one, which is 2.9wt%C and 9.2wt%Cr, since at that moment the right-side part of grain A grows a little faster. Then, grain B successively envelop grain A and complement the solutes around it. Thus at 27.88 s, the interface concentration at the right-side of A is almost unchanged since there is no space there to grow up due to the touching between grain A and B, while is merely 1.6wt%C and 4.2wt%Cr at left-side of A due to its free growth. Thus among 27.00-27.88 s, the right-side part of grain A almost keeps 31 μm from the grain's centreline while its left-side part grows up to 39 μm, with the lacked liquid concentration there. At 27.88 s, the adjacent austenite dendrite B branches up to complete the circling around the grain A, with its dendritic structure changing to a deformed pliers-shaped cluster structure. Besides the single grain's enveloping, several grain's enveloping can also be found in figure 1, as illustrated, the austenite grains G-I contribute together to circle the adjacent M7C3 grain F.

On the contrary, a separate M7C3 carbide grain C and austenite grain D’s growth are shown in figure 3 by tracking the solute concentration distribution along the horizontal centerline of them. As illustrated in figure 3(a)-(b), the solute C and Cr concentrations in M7C3 carbide, which are 8.71wt%C and 44.7wt%Cr, are much higher than those in adjacent liquid. With M7C3 carbide absorbing the solutes during the growth, the concentration at the interface is the lowest during the solute absorption process. Contrastingly, figure 3(c)-(d) shows the solute concentration distribution around a separate austenite grain D, as labelled in figure 1. In this case, the solute concentration in solid is lower than that in liquid, which is consistent with the partition coefficient \( k_{p, \text{L}/\text{L}} < 1 \) for austenite/liquid interface. The austenite rejects the solutes during its growth. Due to the inner dendrite structure of austenite, the uneven concentration distribution is tracked along the horizontal centerline of grain D.

Figure 4 compares the predicted final solidification morphology with the experimental one [3]. Based on the orientation group set for M7C3 carbide and austenite (in section 2.4), the orange to pink-coloured grains represent the M7C3 carbide ones, and the blue to green-coloured grains represent the austenite ones. As seen, the hexagon-shaped M7C3 carbide grains distribute scattered in the austenite matrix, the predicted morphology (figure 4(a)) shows similar to the experimental one (figure 4(b)). Figure 4(c) and 4(d) show the solute concentration profile, the interdendritic structure can be seen there. The predicted average size of M7C3 carbides, measured by Image-pro Plus 6.0, is 71.20 μm, which is fit with the experimental one, 72 μm. And the predicted average solute concentrations in austenite, i.e. the summation of austenite solute mass in all cells divided by the total austenite mass fraction in the region, are 1.61wt%C and 7.87wt%Cr, which are also fit with the predicted concentrations in austenite by solidification path prediction, i.e. 1.64wt%C and 6.63wt%Cr from Gulliver Scheil (GS), 1.65 wt%C and 6.47wt%Cr from lever rule (LR), and 2.04wt%C and 6.87wt%Cr from partial equilibrium (PE) approximation.

Finally, the predicted average liquid concentration evolution during solidification of the Fe-4wt%C-17wt%Cr alloy was checked in Fe-C-Cr alloy liquidus surface phase diagram (figure 5). The averaged liquid concentration is the summation of liquid solute mass in all cells divided by the total liquid mass fraction in the region. As seen, the solidification starts from the liquid+M7C3 regime, then goes directly to FCC regime and finally finishes near the valley between liquid+M7C3 and liquid+FCC regime. The predicted liquid concentration curve by the present model, i.e. the blue-coloured one, shows three turning points, corresponding respectively to the start of the austenite grain precipitation, the touching of the austenite grains with almost all the M7C3 ones, and the accomplishment of the austenite grains enveloping the M7C3 ones. The solidification path prediction by LR, GS and PE prediction are also plotted in the phase diagram. The present prediction fits with them at the initial M7C3 precipitation regime and after the austenite grains' complete enveloping towards the M7C3 grains, returns to overlap the LR, GS and PE prediction curves.
4. Conclusions
A microscopic cellular automaton combined with macroscopic heat and solute transport was developed to simulate the mutual growth and evolution of austenite and M₇C₃ carbide grains during Fe-4wt%C-17wt%Cr ternary alloy solidification process. Results show that,

1) The diffusion of solute C and Cr are contributed together to the constitutional undercooling, together with curvature undercooling for obtaining the grain growth rate of austenite and M₇C₃.

2) Absorption of solute C and Cr to M₇C₃ carbide grain makes its interface the lowest liquid concentration in the region; contrastingly, rejection of solutes from austenite grain makes its interface the higher one. Due to the partition of solutes, the lacked solute concentration is over double of the liquid concentration at M₇C₃/liquid interface, while the accumulated concentration at austenite grain interface is merely one half of its interface liquid concentration.

3) The absorption of solute C and Cr by M₇C₃ grain and rejection of the solutes by austenite grain promote these two grains' cooperative growth. Once they approach to each other, the austenite grain quickly overgrows towards the M₇C₃ grain till finally envelops it.

4) The simulated solidification morphology of the Fe-4wt%C-17wt%Cr alloy, the predicted averaged grain size of M₇C₃ carbides and the C and Cr concentration in austenite grains all agree with the experimental measurements and solidification path prediction. The predicted average liquid concentration curve fits with the LR, GS and PE prediction at the initial M₇C₃ precipitation regime and after the austenite grains' complete enveloping towards the M₇C₃ grains, returns to overlap the LR, GS and PE prediction curves.

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