

Numerical simulation on macrosegregation of ingots with dynamic shrinkage porosity and dendrite microstructure

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Abstract: Macrosegregation and shrinkage porosity are common and interrelated defects that occur during ingot solidification. Existing models typically simulate these phenomena separately rather than in a coupled manner. To address this limitation, this study employed an improved cellular automaton-lattice Boltzmann Method (CA-LBM) model to investigate the mechanisms behind macrosegregation and shrinkage effects during solidification process. Key improvements to the model include the optimization of the migration model in the LBM framework for solid-liquid-gas three-phase mixing to ensure the strict conservation of momentum, mass, and heat, and the incorporation of a shrinkage field during dendrite growth to dynamically track shrinkage evolution. Firstly, the stability and accuracy of the CA-LBM model were validated through simulations of dendrite growth involving coupled multiphysical fields. Subsequently, to investigate the formation mechanisms of macrosegregation and shrinkage porosity defects in both layered and mushy-zone solidification processes, solidification simulations were performed separately for an Fe-0.34wt.%C ingot (layered solidification) and an Al-4.7wt.%Cu alloy ingot (mushy-zone solidification) using the CA-LBM model. For the Fe-0.34wt.%C ingot solidification simulation, the results reveal defects such as axis porosity band, surface sink, hot-top segregation, negative base segregation, A-segregation, and V-segregation. A comparison with simulations that neglect shrinkage effects shows that shrinkage significantly alters both the distribution and morphology of macrosegregation. For the Al-4.7wt.%Cu ingot, the results indicate notable inverse segregation, surface sink, and widespread interdendritic shrinkage. By comparison with scenarios that do not consider shrinkage, it is evident that shrinkage markedly intensifies the degree of inverse segregation.

Keywords: macrosegregation; shrinkage porosity; dendritic morphology; V-segregation; A-segregation

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1 Introduction

In cast products, macrosegregation and shrinkage are two common quality defects^[1-3]. These defects can lead to inhomogeneity in the mechanical properties of castings, making them unable to meet the service requirements. Therefore, it is particularly important to find reasonable casting process parameters to eliminate the defects in the casting process as much as possible. Before the popularization of numerical simulation technology, the selection of process parameters

depends on a large number of experiments, which is time-consuming and costly, and difficult to fully optimize the complex casting process. With the development of computer technology, numerical simulation has become an effective tool for studying the solidification process of castings, which can accurately predict the formation and evolution of defects, significantly reduce the cost of trial and error, shorten the development cycle, and provide technical support for process optimization.

Shen^[1], Li^[2], and Wu^[4] et al. have systematically and comprehensively reviewed the numerical models for ingot macrosegregation. According to Shen's classification criteria, these numerical models can be classified into two categories: (1) macroscopic models (without calculating the microstructure), including multidomain models^[5], continuity models^[6], and

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volume-averaged model^[7]; and (2) quasi-microscopic models (with calculating the virtual dendrite morphology), including two-phase and multiphase models^[8].

Due to the large calculation grid scale of the macroscopic models and the fact that the formation and growth process of microstructure is not considered, the calculated macrosegregation results often have certain errors. In contrast, quasi-microscopic models consider the growth behavior of equiaxed or columnar crystals in the calculation process, which can significantly improve the calculation accuracy. However, the dendritic structure in the quasi-microscopic model is virtually reconstructed and thus exhibits inherent limitations. For example, the model requires artificial assumptions about the morphology of the grains, which are not naturally occurring during ingot solidification. Thus, although the quasi-microscopic model assumes the presence of microstructures, it nevertheless introduces systematic errors in macrosegregation predictions. For example, Ge et al.^[9] used a mixed CET model to calculate quasi-A-segregation bands but failed to predict V-segregation, even though the effect of dendritic morphology (not real secondary dendrite) was taken into account. This shows that although the quasi-microscopic model improves the accuracy of macrosegregation simulation by introducing a virtual microstructure, its intrinsic defects still limit the reliability of macrosegregation prediction. For accurate calculation of macrosegregation, the real dendrite morphology must be considered^[10]. Compared with the model based on virtual microstructure, the model using real microstructure better reflects the physical mechanism of macrosegregation formation. By calculating the real dendritic morphology, not only the accuracy of macrosegregation prediction can be improved, but also a more comprehensive understanding of the complex phenomena during ingot solidification can be achieved.

The study of solidification shrinkage in alloys has been a hot topic since the 1960s. According to Yousefian's^[11] review of the development process, the evolution of solidification shrinkage field can be categorized into four distinct stages: thermal models, thermal/volume calculation models, thermal/fluid flow models, and gas porosity growth models. However, it should be noted that all of these models exhibit certain deficiencies:

(1) The thermal models do not take into account the volume change caused by shrinkage and thus cannot accurately reflect the actual situation of solidification shrinkage.

(2) The thermal/volume calculation models only calculate the total amount of solidification shrinkage but do not involve the dynamic process of shrinkage.

(3) The thermal/fluid flow models treat the skeleton built by dendrites as a porous medium and determine whether gas precipitation occurs in the region near the root of the dendrites by calculating the pressure loss when the melt flows through the porous medium, thus forming micro-shrinkage. However, the model does not consider the dynamic shrinkage process of the dendrite and the melt itself and only takes the change in the

mixing density as the driving factor of the melt flow.

(4) The gas porosity growth models consider the growth and morphology of dendrites in the calculation of microscopic pores formed by gas precipitation. However, the model still fails to describe the dynamic shrinkage process triggered by dendrite growth^[12-16].

Recent studies have proposed numerical models capable of uniformly calculating a variety of shrinkage defects^[17-19], but these models do not involve the calculation of microstructure and macrosegregation, and they fail to describe the shrinkage behavior based on dendrites. During the solidification process, shrinkage occurs in the solid phase represented by dendrites, and the liquid phase represented by the melt. It is imperative to recognize that all shrinkage phenomena are the result of the cumulative effect of shrinkage in each dendrite and the surrounding melt. Consequently, to accurately calculate the shrinkage distribution, it is essential to perform calculations based on dendrites.

In summary, macrosegregation and shrinkage are concurrent phenomena during the solidification process. Therefore, simulating the formation of macrosegregation or shrinkage in isolation clearly cannot fully capture the actual process and lacks sufficient accuracy. Currently, existing models for macrosegregation and shrinkage have certain limitations. To address these limitations, this study developed a coupled CA-LBM model capable of simultaneously calculate solidification shrinkage and macrosegregation. Following model development, validation was performed in two stages: first through quantitative analysis of dendrite tip growth kinetics, followed by demonstration of its accuracy and versatility via simulation of both layered solidification process in Fe-0.34wt.%C ingot and mushy-zone solidification process in Al-4.7wt.%Cu ingot.

2 Mathematic models

The CA nucleation and growth and trapping models used in this study have been validated several times in previous articles of our team, for details please refer to the Refs. [20-22]. The following section details two major enhancements to our previously developed CA-LBM model for alloy ingot solidification.

2.1 Improvements in LBM migration

The cells are classified into four types: a cell with the sum of solid fraction f_s and shrinkage porosity fraction f_k equal to 1 is defined as a solid cell; a cell with $f_k > 0$ and $f_s > 0$ is defined as an interfacial cell (which may also contain shrinkage porosity); a cell with $f_s = 0$ and $f_k > 0$ is defined as a liquid phase cell (which can also have shrinkage porosity); and a cell with $f_k = 1$ is defined as a shrinkage cell. Since the cells in this study involve solid-liquid-gas three-phase mixing problems, direct migration between cells with different liquid phase rates may lead to severe mass, momentum, and heat non-conservation. To ensure strict mass, momentum, and heat conservation, the LBM

model for solute, temperature, and flow fields is modified accordingly, as shown in Fig. 1.

Figure 1 illustrates a schematic diagram of inter-cell migration in the horizontal direction. Since the migration of the melt can only take place in the liquid phase, there is no liquid phase in cell (a), the cell (b) cannot migrate to cell (a). Instead, the migration of material from cell (b) will take place in the liquid phase. At this point, the migrating particles will start from the center of cell (b), rebound after reaching the solid boundary of cell (a), and eventually return to the starting point, with the distance traversed by the particles remains equivalent to the length of a cell. For cell (c), the liquid phase part above the dashed line is the particle that can freely migrate toward cell (b), while the liquid phase part below the dashed line will rebound and return to cell (c) after migrating to the solid boundary of cell (b). Similarly, for cell (d), the liquid phase part above the dashed line can migrate toward cell (c), while the liquid phase part below the dashed line will rebound back to cell (d) after migration.

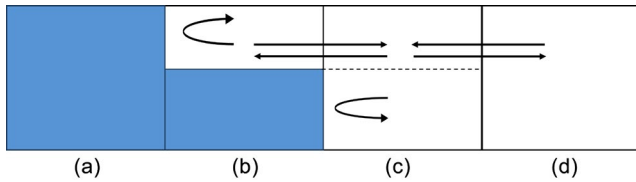


Fig. 1: Corrected schematic of inter-cell migration of LBM:
(a) a cell with $f_i=0$; (b) an interfacial cell with $f_i=0.5$;
(c) a cell with $f_i=0.7$; (d) a cell with $f_i=1$

By this correction mechanism, it is guaranteed that all particles move the same distance in a single time step, thus ensuring the strict conservation of mass, momentum, and heat. The correction mechanism for migration in other directions is the same as that shown in Fig. 1. The LBM equations for the corrected D2Q9 format flow, temperature, and solute fields are, respectively:

$$f_i(x + e_i \Delta t, t + \Delta t) = [1 - f_s(x, t + \Delta t) - f_k(x, t + \Delta t)] \times \left\{ \frac{1}{\tau_f} [f_i^{\text{eq}}(x, t) - f_i(x, t)] + \omega_i \times F(x, t) \right\} + [f_s(x, t + \Delta t) + f_k(x, t + \Delta t)] \times f_{\text{inv}(i)}(x + e_i \Delta t, t) \quad (1)$$

$$g_i(x + e_i \Delta t, t + \Delta t) = [1 - f_s(x, t + \Delta t) - f_k(x, t + \Delta t)] \times \left\{ \frac{1}{\tau_T} [g_i^{\text{eq}}(x, t) - g_i(x, t)] + \omega_i \times H(x, t) \right\} + [f_s(x, t + \Delta t) + f_k(x, t + \Delta t)] \times g_{\text{inv}(i)}(x + e_i \Delta t, t) \quad (2)$$

$$m_i(x + e_i \Delta t, t + \Delta t) = [1 - f_s(x, t + \Delta t) - f_k(x, t + \Delta t)] \times \left\{ \frac{1}{\tau_c} [m_i^{\text{eq}}(x, t) - m_i(x, t)] + \omega_i \times M(x, t) \right\} + [f_s(x, t + \Delta t) + f_k(x, t + \Delta t)] \times m_{\text{inv}(i)}(x + e_i \Delta t, t) \quad (3)$$

The first term on the right side in Eqs. (1–3) is the portion that migrates normally to the neighboring cells, and the second term on the right side is the portion that bounces back during migration. $\text{inv}(i)$ is the particle velocity direction opposite to the direction of i in the D2Q9 model [e.g., $\text{inv}(1)=3$, $\text{inv}(5)=7$] and $f_{\text{inv}(i)}$, $g_{\text{inv}(i)}$, $m_{\text{inv}(i)}$ are the particle distribution functions opposite to the directions of f_i , g_i , and m_i , respectively. $F(x, t)$ is the buoyancy source term in the flow field, and $H(x, t)$ and $M(x, t)$ are the latent heat and mass source terms released by dendrite growth, respectively. $f_i(x, t)$, $g_i(x, t)$, and $m_i(x, t)$ denote the distribution function of the particles in the flow, temperature, and solute fields respectively. τ_f , τ_T , and τ_c are the relaxation times analyzed by Chapman-Enskog^[21].

Fluid density ρ , flow rate u , temperature T , and liquid solutal concentration C_1 can be calculated using the corresponding distribution function, which is given by the following equation:

$$\rho = \sum_{i=0}^8 f_i, \quad u = \frac{\left(\sum_{i=0}^8 f_i \times e_i + \frac{F_b \times \Delta t}{2} \right)}{\rho}, \quad T = \sum_{i=0}^8 g_i, \quad C_1 = \sum_{i=0}^8 m_i \quad (4)$$

2.2 Model of shrinkage field

In CA model, during the growth of dendrites, the shrinkage of solid and liquid phases leads to shrinkage porosity in the cells. The shrinkage rate f_k consists of two components: liquid-phase shrinkage rate f_{kl} and solidification shrinkage rate f_{ks} . Solidification shrinkage is derived by calculating the change in solid-phase rate of the interfacial cells Δf_s in the CA simulation, implying that solidification shrinkage is constantly occurring at the solid-liquid interface during dendrite growth. Specifically, Δf_s reflects the continuous solid phase shrinkage at the solid-liquid interface as the dendrite grows. The calculation of f_{kl} is performed when the metastable temperature is 5 K below the liquidus temperature.

$$f_{ks} = \theta_s \times \Delta f_s, \quad f_{kl} = \theta_l \times f_l \quad (5)$$

where θ_s is the solidification shrinkage rate and θ_l is the liquid phase shrinkage rate.

To ensure strict conservation of momentum and mass, in the shrinkage-liquid phase mixing unit, the liquid-phase rate of the metameres decreases when the f_k increases, while the ρ needs to change in proportion to the decrease of f_l , and C_1 changes accordingly.

$$\rho = \frac{\rho \times f_{l0}}{f_l}, \quad C_1 = \frac{C_1 \times f_{l0}}{f_l} \quad (6)$$

where f_{l0} is the liquid phase ratio before CA calculations.

The LBM was used to simulate the dynamic process of shrinkage. During the calculation process, when shrinkage occurs, particles diffuse to the surrounding cells. Under the action of external forces such as buoyancy, the shrinkage manifests itself as an upward movement. At the same time, the liquid phase from the neighboring cells is fed into the cell where shrinkage occurs. This process results in a decrease in f_k and a corresponding increase in f_l , thereby completing the feeding and shrinkage process. The LBM equation for the

shrinkage field is:

$$s_i(x, t + \Delta t) = \begin{cases} [1 - f_s(x, t + \Delta t)] \times \left\{ \frac{1}{2} [s_i^{\text{eq}}(x, t) - s_i(x, t)] + \omega_i \times S(x, t) \right\} \\ f_s(x, t) \geq f_s(x + e_i \Delta t, t) \\ [f_s(x + e_i \Delta t, t + \Delta t) - f_s(x, t + \Delta t)] \times s_{\text{inv}(i)}(x, t) + \\ \left\{ \frac{1}{2} [s_i^{\text{eq}}(x + e_i \Delta t, t) - s_i(x + e_i \Delta t, t)] + \omega_i \times S(x + e_i \Delta t, t) \right\} \\ f_s(x, t) < f_s(x + e_i \Delta t, t) \end{cases} \quad (7)$$

where $s_i(x, t)$ denotes the distribution function of the shrinkage field and $S(x, t)$ is the external force on the corresponding volume of the shrinkage cell, which is given by:

$$S(x, t) = \rho \times f_k \times g \quad (8)$$

In Eq. (7), the LBM equation for the shrinkage field is discussed in two cases: one where the f_s of the local cell is greater than or equal to that of the neighboring cell, and the other where the f_s of the local cell is less than that of the neighboring cell. The migration of the shrinkage field occurs only in the non-solid region, so the coefficient in Eq. (7) represents the difference in f_s between the cells. In the first case, distribution function is free to migrate to the neighboring cells. After the migration is completed, f_k in the neighboring cell increases while f_i decreases. In the second case, the missing f_s of this cell, compared to its neighbors, will bounce back. Thus, the left-hand side of the equation represents the shrinkage that bounces back to the home cell after migration, while the right-hand side represents the shrinkage successfully migrates into the neighboring cell.

3 Simulation results and discussion

3.1 Model verification

In this section, the Al-4.7wt.%Cu dendrite growth was verified by the interaction of multiple physical fields such as solute, shrinkage, flow, and temperature fields. The computational domain was 200×200 , the grid size was $5 \mu\text{m}$, the initial supercooling was 4.5 K; the thermal boundary conditions of Zhu et al.^[23] were used for heat dissipation, and the solute, shrinkage, and flow field boundaries were treated in half-step bounce format. The physical parameters are shown in Table 1.

Figure 2 shows the solute field, temperature field, and shrinkage field for dendrite growth under gravity natural convection, where the black lines are the flow lines and the arrow direction represents the flow direction.

The average solute concentration is calculated to be 4.699. The theoretical sum of f_k is 407.291, while the actual value is 406.323. The errors in both the solute field and shrinkage porosity field are within 0.3%, indicating that the modified CA-LBM model has good convergence and stability.

As shown in Fig. 2(a), the upper part of the dendrite (upstream tip) is longer than the lower part (downstream tip). To quantitatively analyze the dendrite growth rate, the growth rates of the upstream tip, downstream tip, and horizontal tip were compared with the LGK model. The results of this comparison are presented in Fig. 3.

The dendrite tip growth rate reaches its maximum value at the initial stage, then decreases rapidly before stabilizing at a steady state. Notably, the growth rates vary significantly

Table 1: Physical properties of Al-4.7wt.%Cu and Fe-0.34wt.%C^[22, 24]

Parameters	Symbols	Unit	Value of Fe-0.34wt.%C	Value of Al-4.7wt.%Cu
Melting point	T_m	K	1,811	933.3
Pouring temperature	T_p	K	1,785	917
Solid density	ρ_s	$\text{kg} \cdot \text{m}^{-3}$	7,321	2,743
Liquid density	ρ_l	$\text{kg} \cdot \text{m}^{-3}$	7,027	2,606
Liquidus slope	m_l	$\text{K} \cdot \text{wt.}\%^{-1}$	-84.53	-3.44
Equilibrium partition coefficient	k	/	0.289	0.145
Specific heat	C_p	$\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$	808.254	1,179
Latent heat	L	$\text{J} \cdot \text{kg}^{-1}$	256,476	3.97×10^5
Liquid viscosity	ν	$\text{kg} \cdot \text{m}^{-1} \cdot \text{s}^{-1}$	3.6×10^{-3}	1.3×10^{-2}
Diffusion coefficient	D	$\text{m}^2 \cdot \text{s}^{-1}$	2×10^{-8}	3×10^{-9}
Solutal expansion coefficient	β_c	$\text{wt.}\%^{-1}$	1.1	9.2×10^{-3}
Thermal expansion coefficient	β_T	K^{-1}	2×10^{-3}	10^{-4}
Liquid phase shrinkage rate	θ_l	%	1.6	2
Solidification shrinkage rate	θ_s	%	3	3

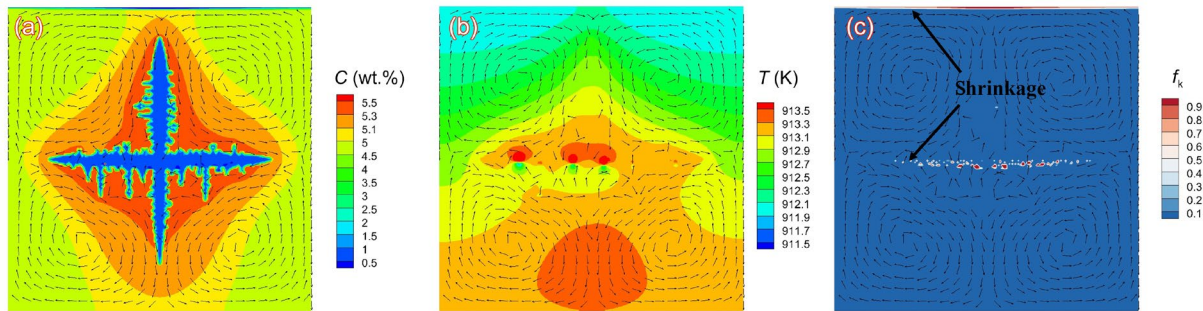


Fig. 2: Diagram of Al-4.7wt.%Cu dendrite: (a) solute field; (b) temperature field; (c) shrinkage field

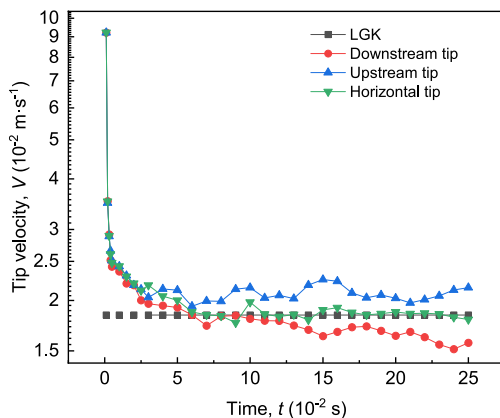


Fig. 3: Al-4.7wt.%Cu dendrite tips growth rate

depending on tip location: the downstream tip shows the slowest growth rate, the upstream tip displays the fastest growth, while the horizontal tip exhibits an intermediate growth rate. This spatial variation in growth kinetics is predominantly governed by convective effects. The interplay of solute convection, thermal convection, and shrinkage-induced convection generates four axisymmetric circulating flows between adjacent dendritic arms, as shown in Fig. 2. The convective transport directs solute and heat toward the bottom region, creating conditions that suppress the growth rate at downstream tips. Conversely, the upstream tips experience enhanced growth rates due to lower local temperatures. The horizontal growth rate, being influenced by both downstream and upstream conditions, shows excellent agreement with theoretical predictions. In Fig. 2(c), shrinkage porosity predominantly accumulates in the upper region as a consequence of feeding and solidification shrinkage processes. In contrast, the porosity formed in the lower section becomes entrapped by secondary dendrite arms and accumulates within interdendritic spaces. This distribution pattern corresponds well to the characteristic porosity formation observed in secondary dendrite arms structures^[15].

In this section, the stability and accuracy of the dendrite growth and multiphysics field model are further demonstrated by validating the growth rate of the dendrite.

3.2 Simulation of Fe-0.34wt.%C solidification

Computational domain of the Fe-0.34wt.%C ingot was divided into $600 \times 1,500$ square cells, each with a length of $50 \mu\text{m}$. The top was considered to be an adiabatic boundary condition

due to the slag insulation^[25], and the bottom and side heat dissipation rate was $700 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$. The half-step bounce format was utilized for the calculation of solute, shrinkage, and flow field boundary conditions. The physical parameters of the alloy are delineated in Table 1.

Figure 4 illustrates the evolution process of solute distribution and streamlines. Observing Fig. 4(a), it can be found that the convection direction at the solid-liquid interface is upward, while the solute discharged by solidification moves upward under the effect of convection. As demonstrated in Fig. 4(b), a high concentration of solutes flows through the region of solidification as they move in an upward direction. Consequently, the concentration of solid solutes in this region is higher. This phenomenon leads to the formation of A-segregation. Due to solute-thermal convection, solutes move upward at the solid-liquid boundary and downward at the core. This results in the downward movement of solutes originally at the top, as illustrated in Fig. 4(c). Consequently, V-shaped solute-enriched zones are formed, as shown in Fig. 4(d). As solidification progresses, these zones evolve into V-segregation. In summary, A-segregation and V-segregation are caused by solute-thermal convection, which is in agreement with the result from Asai et al^[26]. As shown in Fig. 4(e), solute migrates from the bottom to the top of the ingot under convective flow, resulting in solute depletion at the bottom and enrichment at the top. This transport mechanism leads to the formation of negative base segregation. By analyzing the streamline distribution in the top region, it can be found that a vortex structure is formed in this region, which makes the solute circulate in the local region of the top without diffusing downwards. The vortex-induced solute accumulation further promotes the development of hot-top segregation, as demonstrated in Fig. 4(f).

Figure 5 shows the evolution process of microstructure and streamline for Fe-0.34wt.%C ingot. In the early stage of solidification, the dendrites grow mainly along the direction perpendicular to the boundary shown in Fig. 5, due to that the heat dissipation rate is maximum in this direction. The solidification of the ingot shows a planar solidification pattern from the outside to the inside, while the melt at the top flows downward to compensate for internal shrinkage within the ingot, resulting in surface sink at the top. However, Fig. 5(d) reveals that the planar dendritic growth pattern in the top region becomes disrupted. This breakdown occurs

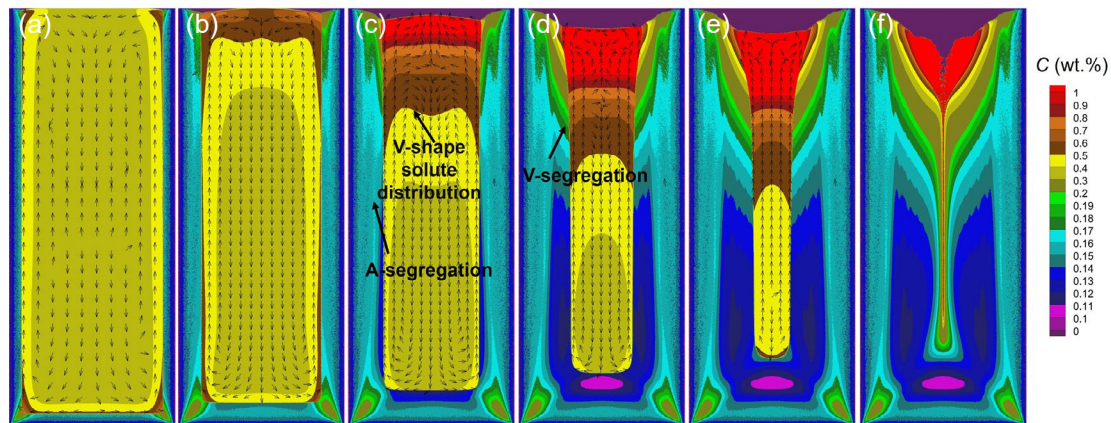


Fig. 4: Solute field evolution for Fe-0.34wt.%C ingot: (a) 2 s; (b) 6 s; (c) 12 s; (d) 25 s; (e) 40 s; (f) 70 s

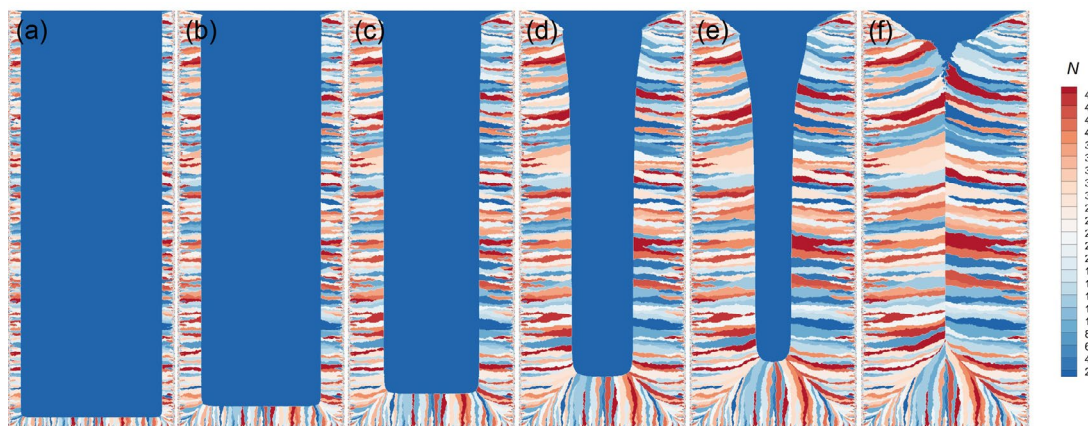


Fig. 5: Dendrite morphology evolution for Fe-0.34wt.%C ingot: (a) 2 s; (b) 6 s; (c) 12 s; (d) 25 s; (e) 40 s; (f) 70 s

because solute enrichment at the top [Fig. 4(d)] increases the constitutional supercooling requirement for dendritic growth. Consequently, the growth rate of top dendrites decreases significantly compared to those in the middle and lower regions, resulting in markedly shorter dendritic lengths in the upper zone. In addition, at the solid-liquid interface, the growth direction of the dendrites gradually changes from perpendicular to the wall to obliquely upward due to the continuous upward solute-thermal convection.

Figure 6 shows the temperature field evolution process for Fe-0.34wt.%C ingot. It can be observed that the isotherms in Figs. 6(a) and (b) are basically parallel to the boundary. However, in Figs. 6(c) and (d), the isotherms at the growth interface at the top of the ingot show inward curve, i.e., the temperature near the top boundary of the ingot is lower than that in its middle region on the same vertical line. This is primarily attributed to the slower dendrite growth rate at the top relative to the center in the middle and late solidification stages, which reduces latent heat release and results in a lower temperature.

Figure 7 shows the dynamic evolution process of the shrinkage field for Fe-0.34wt.%C ingot. In Fig. 7(a), a thin layer of shrinkage bands is formed at the solid-liquid interface due to solidification shrinkage induced by dendrite growth. In Fig. 7(b), the shrinkage band gradually coarsens under the influence of feeding and its position moves upwards. At the same time, as the shrinkage continues to move upwards,

surface sinking gradually occurs at the top of the ingot. This phenomenon visualizes the dynamics of the liquid steel flow during solidification and its effect on the ingot. Figure 7(c) demonstrates liquid-phase shrinkage occurring in the core region of the ingot. This phenomenon results from liquid-phase shrinkage as the core temperature decreases during solidification. This observation is in agreement with the findings of Khalajzadeh et al.^[17]. Meanwhile, the surface sink further expands with the increase of liquid phase shrinkage in the core. In Figs. 7(d) and (e), as the solidification rate of the ingot gradually slows down, the shrinkage process also decelerates. With the progression of the solid-liquid interface, the surface sink takes on an inverted triangular conical shape. By the stage shown in Fig. 7(f), the remaining liquid phase in the ingot has fully transformed into a solid phase. In these final solidification regions, the significant reduction in the liquid-phase makes the feeding process exceptionally difficult, resulting in the formation of a significant shrinkage cavity in these areas.

In Fig. 8(a), it can be found that the shrinkage is primarily characterized by an inverted triangular surface sink, concentrated shrinkage cavities, and axial porosity bands. A-segregation, V-segregation, hot-top segregation, and negative base segregation are evident in Fig. 8(c). The distribution of shrinkage and macrosegregation in Figs. 8(a) and (c) fits well with the distribution of common defects in carbon steel ingots.

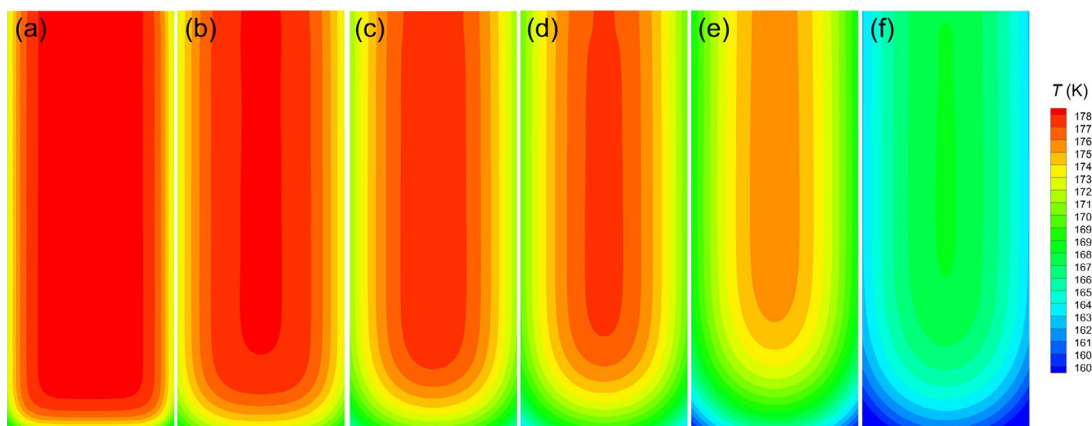


Fig. 6: Temperature field evolution for Fe-0.34wt.%C ingot: (a) 2 s; (b) 6 s; (c) 12 s; (d) 25 s; (e) 40 s; (f) 70 s

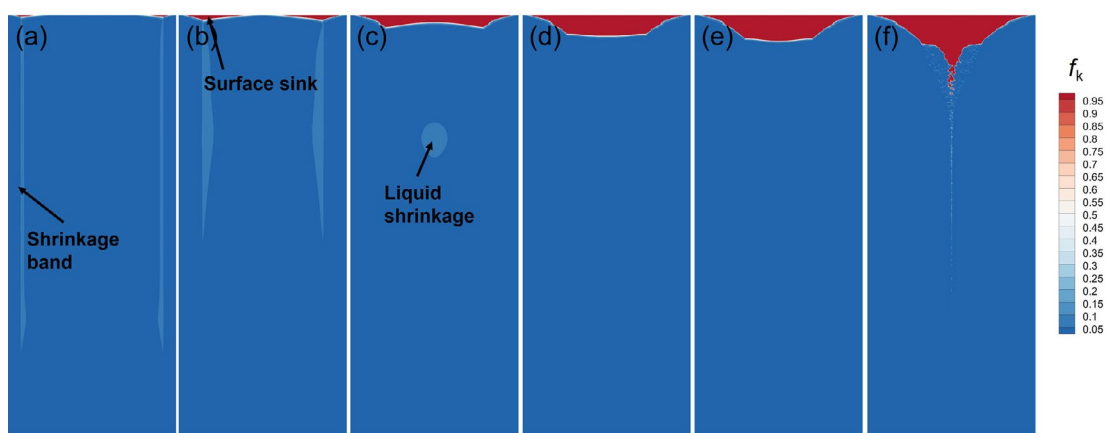


Fig. 7: Shrinkage field evolution for Fe-0.34wt.%C ingot: (a) 2 s; (b) 6 s; (c) 12 s; (d) 25 s; (e) 40 s; (f) 70 s

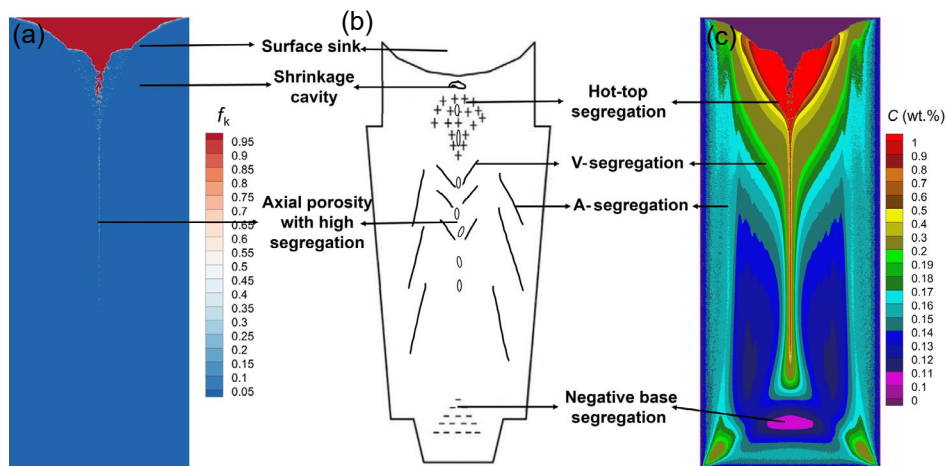


Fig. 8: Shrinkage field (a), shrinkage and macrosegregation defects distribution (b)^[1, 2], and solute field (c)

Figure 9 shows the macrosegregation distribution of Fe-0.34wt.%C ingots without and with shrinkage under the same solidification conditions. The results show that both scenarios (with and without shrinkage) exhibit A-segregation, V-segregation, negative base segregation, and hot-top segregation. However, the specific distribution pattern of segregation differs in the two cases.

In the lower half of the Zone I, the width of the A-segregation narrows significantly with shrinkage, while its position shifts inward. The length of A-segregation in the

upper half is also significantly shortened. This is because, at the beginning of solidification of the ingot, the sidewall region discharges solute outwards, forming a high concentration solute mass moving upwards, and after the introduction of the shrinkage field, as shown in Fig. 7(a), an upward shrinkage band is also formed at the sidewall, whose trajectory coincides with the trajectory of the high concentration solute mass. This coupling significantly changes the formation process of A-segregation, which in turn has a significant effect on its distribution.

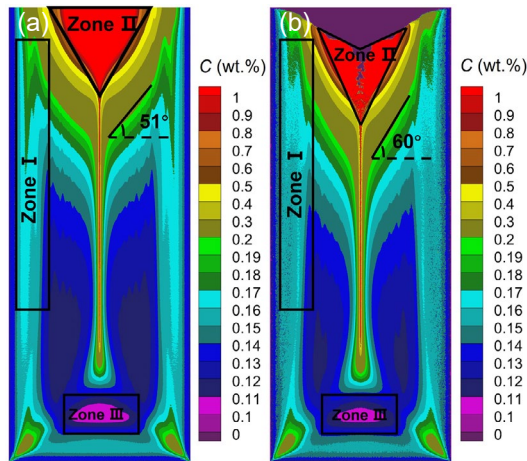


Fig. 9: Solute field for Fe-0.34wt.%C ingot: (a) without shrinkage; (b) with shrinkage

The hot-top segregation region in Zone II is significantly affected by shrinkage. As shown in Figs. 9(a) and (b), the surface sink replaces the original hot-top segregation region, causing a notable downward shift of Zone II when shrinkage is accounted for. Additionally, quantitative analysis of Zone II shows that the area of segregation decreases by approximately 32.6%, while the average solute concentration increases by about 62.8%. This result suggests that solidification shrinkage not only causes a downward shift in the top positive segregation position but also reduces the area of the top positive segregation region and significantly enhances the degree of segregation.

The area of negative base segregation in Zone III remains almost unchanged. A quantitative analysis of its solute distribution reveals that the average solute concentration in Zone III has increased by 8.3% in Fig. 9(b) compared with Fig. 9(a). This phenomenon is due to the fact that the negative base segregation region is formed during the early solidification of the ingot, and therefore its distribution is less affected by shrinkage. Meanwhile, the overall concentration of the liquid phase of the ingot rises due to the shrinkage effect, which in turn attenuates the degree of negative base segregation.

The V-segregation is formed in the middle stage of solidification, and the surface sink is more obvious, so the overall position of the V-segregation is shifted downward under the effect of shrinkage. At the same time, the V-segregation is formed gradually from outside to inside and from top to bottom during the solidification process. As shown in Fig. 4(c), on the outer side of the ingot, the V-segregation starts to form when the surface sink is not yet fully formed, so the distribution of the V-segregation zone that near the ingot boundary is basically the same as that of Fig. 9(a); whereas in Fig. 4(e), the melt has dropped significantly when the end part of the V-segregation is formed. As a result, the V-segregation in Fig. 9(b) is more downward at the center area compared with Fig. 9(a), and the segregation angle also increases from 51° to 60° . This phenomenon further verifies that solidification shrinkage has a significant effect on the macrosegregation pattern.

According to the above discussion, shrinkage significantly affects the distribution, degree, and pattern of macrosegregation in Fe-0.34wt.%C ingots. Under the shrinkage field, the A-segregation area narrows and shifts inward. In Zone II, the surface sink effect causes a significant downward shift of the hot-top segregation and a significant increase in the degree of segregation. In contrast, the negative base segregation distribution area is almost unaffected by shrinkage in Zone III, the degree of segregation has been slightly reduced. The downward shift of V-segregation and the increase in the angle demonstrate the effect of solidification shrinkage on the macrosegregation pattern. Overall, solidification shrinkage not only affects the distribution of macrosegregation, but also significantly changes the pattern and degree of segregation in Fe-0.34wt.%C ingots.

3.3 Simulation of Al-4.7wt.%Cu solidification

In this section, the bottom and side heat dissipation rate is $500 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, while the top is considered an adiabatic boundary condition due to the slag insulation^[25]. The ingot geometry and boundary conditions remain consistent with those described in Section 3.2. The physical parameters of the alloy are shown in Table 1.

Figure 10 illustrates the evolution of the solute field, dendrite morphology, and streamlines during the ingot solidification process. By analyzing the flow streamlines, it is observed that in Fig. 10(a) the boundary region develops downward flow while upward flow dominates in the core region, establishing two large circulations. This characteristic flow pattern emerges due to solutal-thermal convection during the initial solidification phase. As dendrites grow in Fig. 10(b), their arms obstruct convection, reducing the recirculation zones while disordered convective flows emerge between dendrite arms. By Fig. 10(d), further dendrite growth diminishes the recirculation vortices and causes visible distortion in convection patterns, with the melt developing irregular flow pathways through the dendrite arm network. Finally, in Fig. 10(e), when the liquid-phase region in the ingot almost completely disappears, the irregular convection is only retained in the region of the melt divided by the dendrites.

At the initial stage of solidification [Figs. 10(a) and (b)], the solute discharged at the solid-liquid interface is transported to the bottom of the ingot by downward convection, while the melt confined between the dendrite arms has limited flow. Meanwhile, the solute near the core is drawn to the top by upward convection. As the solidification process progresses, secondary dendrite arms form, making it more difficult for the solutes trapped between the dendrites to flow out. In Figs. 10(c), (d), (e), and (f), as the solid-liquid interface continuously advances inward toward the core region, the solute accumulated in the core migrates toward the boundary along the direction of downward convection. It is evident that the solute concentration at the bottom and side boundary is significantly higher than at the core, indicating the occurrence of inverse segregation.

As for dendrite morphology, the evolution process is characterized by different growth patterns: initially in Fig. 10(a), columnar dendrites grow orthogonally to the boundary surface, while in Fig. 10(b), the primary dendrite at the top exhibits slower growth due to solute enrichment near the upper region and the influence of surface sink, while secondary dendrite arms begin to develop. As seen in Fig. 10(c), both primary and secondary dendrite arms continue to grow, but the primary dendrite length becomes significantly shorter at the top compared to those in the middle and lower parts. In Figs. 10(e) and (f), the dendrites extend to the ingot core, restricting further growth along their preferred orientation. Consequently, they grow at nearly isotropic rates, leading to dendrite coarsening and the formation of tertiary dendrite arms.

Figures 11 show the temperature field evolution process during solidification process of Al-4.7wt.%Cu. The isotherms in Fig. 11(a) are parallel to the boundary. In Fig. 11(c), the isotherms at the top show an inward depression due to lower dendrite growth rate in this region. This slower growth releases less latent heat, leading to lower temperatures. Subsequently, as cooling proceeds, the overall temperature of the ingot continues to decrease, as shown in Figs. 11(d), (e), and (f).

Figure 12 demonstrates the shrinkage field evolution during solidification of Al-4.7wt.%Cu alloy. At the initial stage of solidification [Figs. 12(a) and (b)], dendrite growth causes solidification shrinkage at the solid-liquid interface, which in turn induces the melt at the top to compensate for

the shrinkage, resulting in surface sink. Due to the high solid phase ratio and low liquid phase ratio between the dendrites, the feeding process is limited^[27], leading to interdendritic shrinkage. As shown in Figs. 12(d) and (e), progressive dendrite growth isolates liquid-phase regions, terminating liquid compensation and forming distinct interdendritic shrinkage zones. Notably, in Fig. 12(f), the spatial distribution of shrinkage porosity exhibits marked differences, with more severe formation along sidewalls compared to the bottom region. This variation stems from distinct solidification conditions: vertically oriented primary dendrites at the bottom maintain liquid connectivity with the core during initial solidification, enabling effective feeding. Consequently, the bottom develops discrete point-like shrinkage, while sidewalls form continuous tubular shrinkage along columnar dendrite boundaries^[28, 29].

To compare the effect of shrinkage on segregation in Al-4.7wt.%Cu ingots, the solidification of ingots without shrinkage was simulated. The solute distribution of the ingots with and without shrinkage is shown in Fig. 13, and Fig. 14 shows the average solute concentration for each zone.

In Fig. 14, the average solute concentrations in Zones I, II, III, and IV at the ingot boundary are higher than those in Zones V, VI, and VII at the core. This is primarily due to the convective effect, which drives solutes in the ingot core to migrate toward the boundary, leading to a decrease in core concentration. As a result, inverse segregation occurs. It is worth noting that inverse segregation occurs whether or not shrinkage effects are considered.

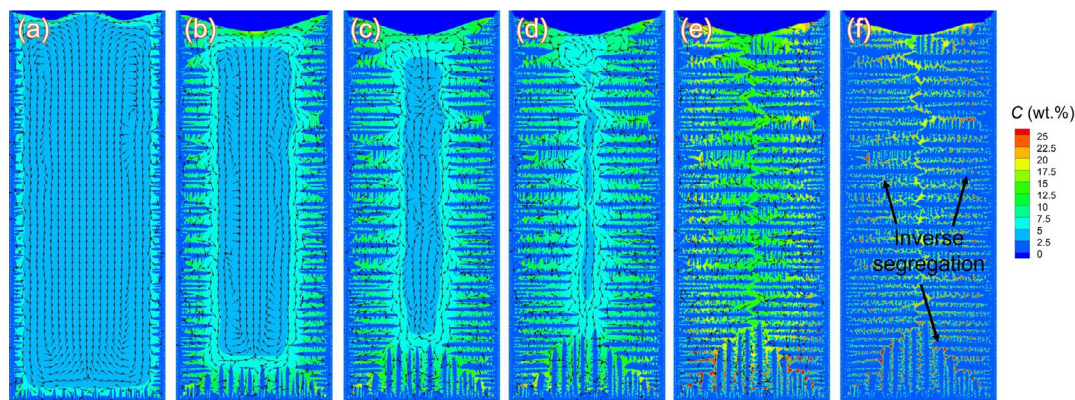


Fig. 10: Solute field evolution for Al-4.7wt.%Cu ingot: (a) 2 s; (b) 7 s; (c) 15 s; (d) 30 s; (e) 50 s; (f) 110 s

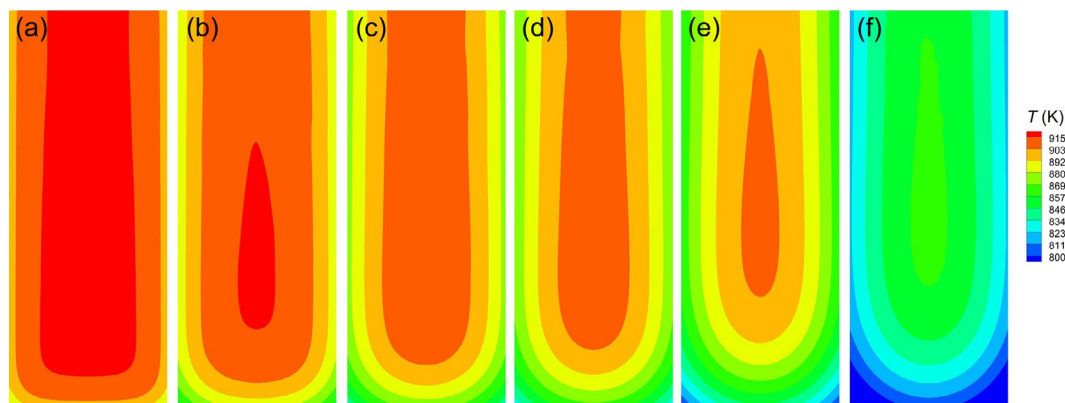


Fig. 11: Temperature field evolution for Al-4.7wt.%Cu ingot: (a) 2 s; (b) 7 s; (c) 15 s; (d) 30 s; (e) 50 s; (f) 110 s



Fig. 12: Shrinkage field evolution for Al-4.7wt.%Cu ingot: (a) 2 s; (b) 7 s; (c) 15 s; (d) 30 s; (e) 50 s; (f) 110 s

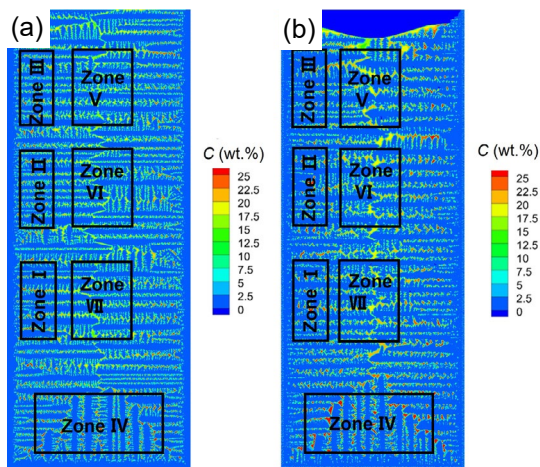


Fig. 13: Solute field for Al-4.7wt.%Cu ingot: (a) without shrinkage; (b) with shrinkage

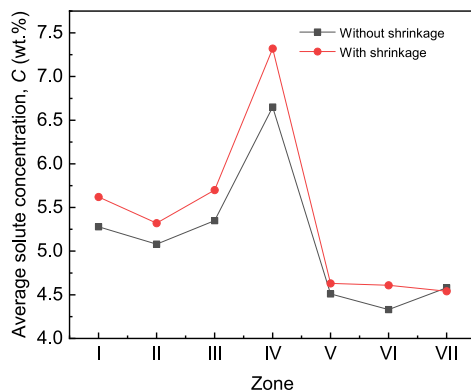


Fig. 14: Comparison of average solutes of Al-4.7wt.%Cu ingot in different zones with and without shrinkage

By comparing the average solute concentrations for the two different cases in Fig. 14, it is found that the shrinkage effect significantly enhances the degree of inverse segregation in most zones. For example, the average solute concentration in Zone IV increases by about 10.1%, while in Zone III, it increases by about 6.5%. In contrast, in Zone VII, the average concentration decreases by about 0.9%. These changes indicate that the shrinkage effect not only exacerbates inverse segregation but also has a differential impact across different zones.

Theoretically, the average concentration should increase by about 5.26% under shrinkage. However, the rate of change in the boundary regions typically exceeds 5.26%, especially in Zone IV. This suggests that the enhancement of inverse segregation is not solely due to the increase in average solute concentration caused by shrinkage, but also stems from the fact that shrinkage alters solute transport behavior, leading to a greater accumulation of solutes near the boundary. Collectively, these results demonstrate that the shrinkage effect significantly exacerbates inverse segregation, particularly at the boundary.

4 Conclusions

The CA-LBM model was modified by introducing a bounce-back mechanism during the migration of distribution functions between cells with varying liquid fractions, thereby ensuring strict conservation of mass, momentum, and heat. Additionally, a shrinkage model was incorporated into the dendrite growth process, enabling dynamic tracking of shrinkage during solidification and coupled computation of macrosegregation and shrinkage porosity. The stability and accuracy of the CA-LBM model were then validated using coupled multiphysics fields to calculate the growth rate of Al-4.7wt.%Cu dendrites. Following conclusions can be achieved:

(1) The CA-LBM model developed in this study has successfully simulated the layered solidification process in Fe-0.34wt.%C ingots, providing insights into the formation mechanisms of defects under the coupled evolution of macrosegregation and shrinkage. The results demonstrate that macrosegregation formation is primarily governed by solute-thermal convection and solid-liquid interface interactions. Furthermore, when shrinkage effects are incorporated, the overall macrosegregation severity in the ingots is found to increase significantly.

(2) Numerical simulation of the mushy-zone solidification process in Al-4.7wt.%Cu ingots successfully elucidates the formation mechanisms of both inverse segregation and shrinkage defects. The results demonstrate that inverse segregation primarily stems from solute-thermal convection

at the solid-liquid interface, leading to solute depletion in the core region. Furthermore, interdendritic shrinkage porosity develops when liquid feeding becomes restricted by secondary dendrite arms. In contrast to Fe-0.34wt.%C ingots, the incorporation of shrinkage effects in Al-Cu alloys leads to significant intensification of inverse segregation at the bottom while producing relatively minor effects along the sidewalls.

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Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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