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Cellular Automaton Simulation of Solidification Microstructure in Ductile Iron: A Postprint

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Abstract

An improved multi-phase cellular automaton (MCA) model, built upon previous work, was developed to simulate the microstructure evolution of ductile iron solidifying via the divorced eutectic mechanism. The model employs a local solute equilibrium method to calculate the growth kinetics of graphite and austenite, and incorporates the density ratio of graphite to Fe in the graphite growth model. This model can reproduce microstructural morphologies that are consistent with experimental observations. The model was applied to simulate and analyze the interaction and competitive growth mechanisms between graphite and austenite, discuss the influence of cooling rate on the size and size distribution of graphite nodules at the end of solidification, and compare the simulation results with experimental data. The results indicate that austenite precipitation promotes the growth of neighboring graphite in the liquid phase; the growth of both austenite and graphite phases is controlled by C diffusion; and the growth rate of graphite slows down when it is surrounded by austenite. Furthermore, as the cooling rate increases, the solidification time decreases, the average radius of graphite nodules decreases, and the variation pattern of graphite nodule size distribution under different cooling rate conditions shows good agreement with experimental results.

Full Text

1.1 Model Description

This work investigates the interaction and competitive mechanisms between spheroidal graphite and austenite phases, as well as the evolution of the concentration field during the divorced eutectic solidification of hypereutectic spheroidal graphite cast iron. The two-dimensional computational domain is discretized into uniform square cells. In this three-phase system comprising liquid, austenite, and graphite, each cell is assigned variables including composition, temperature, volume fractions of the three phases (liquid, austenite, and graphite), preferred orientation of austenite dendrites, graphite nodule identification numbers, and cell states: liquid (fL=1), graphite (fGr=1), austenite (fg=1), graphite/liquid interface (0<fGr<1, fg=0), graphite/austenite interface (0<fGr<1, fL=0), austenite/liquid interface (0<fg<1, fGr=0), and graphite/austenite/liquid interface (fGr>0, fg>0, fGr+fg<1), where fL, fGr, and fγ represent the volume fractions of liquid, graphite, and austenite, respectively.

At the beginning of simulation, all cells in the domain are initialized with uniform composition and temperature, starting from the liquidus temperature corresponding to the initial composition. For hypereutectic spheroidal graphite cast iron, graphite precipitates from the liquid when the temperature falls below the graphite liquidus temperature and grows in a nearly spherical shape. When the temperature reaches the eutectic temperature, austenite precipitates and grows together with graphite in a divorced eutectic manner. The nucleation densities of graphite and austenite are determined based on nucleation models from literature [18] or relevant experimental data. After nucleation, the positions of graphite and austenite remain fixed, neglecting any flotation effects caused by fluid flow. During solidification, when graphite contacts austenite, it is rapidly enveloped by an austenite shell and continues to grow by absorbing solute carbon from the surrounding austenite until the simulation ends at the eutectoid temperature. Austenite grows continuously, rejecting solute carbon into the surrounding liquid until the austenite shells impinge, completing solidification. This model neglects the effect of fluid flow on solute transport, with carbon diffusion occurring purely by diffusion. The temperature is assumed to be uniformly distributed throughout the computational domain and cools at a constant rate, where the cooling rate is influenced by both heat extraction and latent heat release during graphite and austenite growth.

The growth kinetics of graphite and austenite are calculated using the local solute equilibrium model [17], where the driving force for growth is a function of the difference between the interfacial equilibrium composition and the actual composition. The local interfacial equilibrium composition is calculated based on local temperature and interfacial curvature, while the actual composition is obtained from the concentration field calculation. Additionally, this model incorporates the density ratio between graphite and Fe in the growth calculations.

1.2 Concentration and Temperature Field Calculations

Solute equilibrium is assumed at the austenite/liquid, graphite/liquid, and graphite/austenite interfaces. On one hand, austenite rejects solute into the surrounding liquid during growth, and solute redistribution at the solid/liquid interface is calculated according to the equilibrium partition coefficient kγ. On the other hand, graphite absorbs solute carbon from the surrounding liquid or austenite phase during growth. The combined effect creates concentration gradients ahead of the growth interface, driving carbon diffusion. The solute transport governing equation accounting for solute redistribution is:

$$\frac{\partial C_i}{\partial t} = \nabla \cdot (D_i \nabla C_i) + \frac{\partial f_\gamma}{\partial t} \frac{(C_i^* - C_\gamma^*)}{1 - f_\gamma - f_{Gr}} - \frac{\partial f_{Gr}}{\partial t} \frac{(C_{Gr} - C_i^*)}{1 - f_\gamma - f_{Gr}}$$

where t is time, Ci is composition, Di is the diffusion coefficient, subscript i denotes austenite (γ) or liquid (L) phase, Ci* is the composition of austenite at the graphite/austenite interface or the liquid composition at graphite/liquid and graphite/austenite/liquid interfaces, and CGr is the carbon content in graphite (CGr=100%). The second term on the right side represents solute redistribution at the austenite/liquid or austenite/graphite/liquid interface during austenite growth, implemented by adding the rejected solute to the remaining liquid in the same interfacial cell. If the interfacial cell is fully solidified at that time step, the rejected solute is added to adjacent liquid cells. The third term represents solute redistribution at the graphite/liquid, graphite/austenite, or graphite/austenite/liquid interface during graphite growth, implemented by subtracting the absorbed solute from the remaining liquid or austenite in the same interfacial cell. If the interfacial cell has fully transformed to graphite at that time step, the absorbed solute is subtracted from adjacent liquid or austenite cells.

The simulation system includes three distinct phases (liquid, graphite, and austenite) and four different interfaces (austenite/liquid, graphite/liquid, graphite/austenite, and graphite/austenite/liquid), where carbon composition and diffusion coefficients vary significantly. To effectively handle the discontinuities in carbon composition and diffusion coefficients at interfaces, an effective composition Ce and effective diffusion coefficient De are employed when solving the diffusion equation. For example, the effective compositions for liquid and austenite are Ce=CL and Ce=Cγ/kγ, respectively, while the effective diffusion coefficients are De=DL and De=Dγ. For graphite and its adjacent phases, the effective diffusion coefficient is Ce=0 because graphite has an equilibrium composition of 100% C. Although the concentration difference between graphite and its surrounding liquid or austenite is substantial, their chemical potentials are equal according to phase equilibrium principles, preventing carbon diffusion from graphite to liquid or austenite. Detailed determination methods for cell types and equilibrium concentrations in different cell types are described in literature [19].

Equation (2) is discretized and solved using an explicit finite difference method with no-flux boundary conditions. The stable time step Δt is determined by the carbon diffusion coefficient in liquid and mesh size Δx:

$$\Delta t = \frac{\Delta x^2}{4D_L}$$

During solidification, heat exchange with the mold causes temperature decrease, providing the driving force for solidification, while phase transformation releases latent heat, causing temperature increase. The combined effect makes the system temperature vary with solidification time. Although temperature distribution and state vary at different positions within the casting at different temperatures, the simulation domain is relatively small, and the thermal diffusivity of Fe-C alloys is approximately three orders of magnitude larger than the diffusion coefficient of carbon in liquid. Therefore, this model assumes uniform temperature distribution within a micro-region, with temperature influenced by both heat extraction and latent heat release, calculated as:

$$T = T_0 + \dot{T}t - \frac{L_{V,\gamma}\Delta f_\gamma + L_{V,Gr}\Delta f_{Gr}}{\rho c_p}$$

where $\dot{T}$ is the heat extraction rate, representing the temperature decrease rate due to heat exchange with the mold, which can be determined by fitting cooling curves before and after phase transformation;   is the density of Fe; cp is the specific heat capacity of Fe; and LV,γ and LV,Gr are the volume latent heats of austenite and graphite, respectively.

1.3 Graphite Growth Model

During spheroidal graphite cast iron solidification, graphite growth occurs in two stages: growth in liquid and growth within the austenite shell after being enveloped. As mentioned, the local solute equilibrium model [17] is employed to calculate graphite growth, with the driving force being the difference between local interfacial equilibrium composition and actual composition. When graphite grows in liquid, interfacial curvature effects must be considered, and the equilibrium composition at the graphite/liquid interface is calculated as:

$$C_{eq}^{Gr/L} = C_0 + \frac{T^* - T_{eq}^{Gr/L}}{m_{L,Gr}} + \frac{\Gamma_{Gr} K_{Gr/L}}{m_{L,Gr}}$$

where T* is the interfacial temperature, $T_{eq}^{Gr/L}$ is the equilibrium temperature corresponding to the initial composition C0, mL,Gr is the liquidus slope of graphite, KGr/L is the curvature of the graphite/liquid interface, and ΓGr is the Gibbs-Thomson coefficient of graphite. In this 2D model, the average curvature of the graphite interface is calculated as:

$$K_{Gr/L} = \frac{1}{\sqrt{V_C f_{Gr}^{sum}}}$$

where VC is the area of each cell and f_{Gr}^{sum} is the sum of graphite volume fractions belonging to the same graphite nodule. Based on interfacial solute conservation and considering the density difference between graphite and Fe, the increment of graphite volume fraction ΔfGr in a graphite/liquid interfacial cell during one time step is:

$$\Delta f_{Gr} = \frac{D_L G_{Gr}(C_i^* - C_{eq}^{Gr/L})\Delta t}{\rho_{Gr}(1 - C_i^*)}$$

where Gr is the density of graphite, Ci* is the composition at the graphite/liquid interface obtained from the concentration field calculation, and GGr is a geometry factor related to neighboring cell states, determined by:

$$G_{Gr} = \begin{cases} \min\left(1, \frac{\sum_{m=1}^{4} S_I^m + \frac{1}{\sqrt{2}}\sum_{n=1}^{4} S_{II}^n}{f_{Gr}^{sum}}\right) & \text{if } f_{Gr} < 1 \\ 1 & \text{if } f_{Gr} = 1 \end{cases}$$

where SI represents the state parameters of the four nearest neighbor cells and SII represents the state parameters of the four second-nearest neighbor cells. The geometry factor GGr accounts for the influence of neighboring graphite cells on the growth of graphite in the current cell, considering that nearest neighbors have greater influence than second-nearest neighbors due to mesh spacing.

When graphite grows within austenite, the calculation method is similar to that for liquid growth, except that $T_{eq}^{Gr/L}$ and mL,Gr in Equation (5) are replaced by the equilibrium temperature $T_{eq}^{Gr/\gamma}$ and solidus slope ms,Gr at the graphite/austenite interface, respectively, and interfacial curvature effects are neglected. Therefore, the equilibrium composition at the graphite/austenite interface $C_{eq}^{Gr/\gamma}$ is calculated similarly to Equation (7). The increment of graphite volume fraction ΔfGr at the graphite/austenite interface during one time step is:

$$\Delta f_{Gr} = \frac{D_\gamma G_{Gr}(\bar{C}_\gamma^* - C_{eq}^{Gr/\gamma})\Delta t}{\rho_{Gr}(C_{Gr} - C_{eq}^{Gr/\gamma})}$$

where $\bar{C}_\gamma^*$ is the local average composition of austenite at the graphite/austenite interface. For a graphite/austenite interfacial cell I, the local average composition is calculated as:

$$\bar{C}_\gamma^*(I) = \frac{C_\gamma^*(I) + \sum_{J=1}^{N} C_\gamma^*(J)}{N+1}$$

where $C_\gamma^*(I)$ is the austenite composition of interfacial cell I, and $C_\gamma^*(J)$ is the sum of austenite compositions of neighboring interfacial cells J, with N being the number of neighboring interfacial cells. The local austenite composition is obtained from the concentration field calculation.

When the graphite volume fraction in a graphite/liquid or graphite/austenite interfacial cell reaches 1, the cell state transforms from an interface cell to a graphite cell, capturing new neighboring graphite/liquid or graphite/austenite interfacial cells to enable continued graphite growth.

1.4 Austenite Growth Model

The local solute equilibrium method [17] is also employed to calculate austenite dendrite growth kinetics, considering preferred growth direction, interfacial curvature variation, and anisotropy of interfacial energy and growth kinetics. The driving force for dendrite growth is the difference between the actual composition and equilibrium composition at the dendrite/liquid interface. When growing in liquid, the equilibrium composition at the austenite/liquid interface is calculated as:

$$C_{eq}^{\gamma/L} = C_0 + \frac{T^* - T_{eq}^{\gamma/L}}{m_{L,\gamma}} + \frac{\Gamma_\gamma K_\gamma \phi}{m_{L,\gamma}}$$

where $T_{eq}^{\gamma/L}$ is the equilibrium temperature at the austenite/liquid interface, mL,γ is the liquidus slope of austenite, Γγ is the Gibbs-Thomson coefficient of austenite, Kγ is the curvature of the austenite/liquid interface calculated using the counting cell method [20], and ϕ is the interfacial energy anisotropy function given by:

$$\phi(\theta_0) = 1 - \delta_t \cos[4(\theta - \theta_0)]$$

where δt is the interfacial energy anisotropy strength, 0 is the preferred dendrite orientation, and   is calculated as:

$$\theta = \arccos\left(\frac{\partial f_\gamma/\partial x}{\sqrt{(\partial f_\gamma/\partial x)^2 + (\partial f_\gamma/\partial y)^2}}\right)$$

Based on interfacial solute balance, the increment of austenite volume fraction Δfγ in an austenite/liquid interfacial cell during one time step is:

$$\Delta f_\gamma = \frac{D_L G_\gamma (C_{eq}^{\gamma/L} - C_i^*)\Delta t}{(1 - C_{eq}^{\gamma/L})\eta}$$

where $C_{eq}^{\gamma/L}$ is the equilibrium composition calculated from Equation (12), Ci* is the actual composition at the austenite/liquid interface obtained from the concentration field calculation, Gγ is the geometry factor calculated similarly to Equation (8) by replacing graphite volume fraction with austenite volume fraction, and   is the interfacial kinetic anisotropy function calculated as:

$$\eta(\theta_0) = 1 + \delta_k \cos[4(\theta - \theta_0)]$$

where δk is the interfacial kinetic anisotropy strength.

When the austenite volume fraction in an austenite/liquid interfacial cell reaches 1, the cell state transforms from an austenite/liquid interfacial cell to an austenite cell, capturing neighboring liquid cells as new austenite/liquid interfacial cells to enable continued austenite growth. When graphite grows within austenite, the increment of graphite volume fraction in a graphite/austenite interfacial cell during one time step equals the decrease in austenite volume fraction.

1.5 Coupling of Graphite and Austenite Dendrite Growth Models

The coupling method integrating graphite and austenite nucleation and growth with concentration and temperature field calculations proceeds as follows: At the beginning of simulation, all cells in the computational domain are initialized with uniform initial composition and temperature. The domain then cools at a certain rate according to the heat extraction rate. Based on the real-time temperature, the model checks whether nucleation conditions for graphite and austenite are satisfied. If satisfied, graphite or austenite nucleates, and nucleated cells are assigned appropriate state values. Multiple interface types coexist during solidification. When austenite grows, the increment of austenite phase fraction is calculated according to Equations (12)-(15). Graphite growth in liquid and within austenite is calculated using Equations (5)-(8) and (9)-(11), respectively. Carbon diffusion and solute redistribution due to phase transformation are calculated according to Equations (1) and (2). As mentioned, this model incorporates the density ratio between graphite and Fe. To ensure solute conservation throughout the computational domain, an equivalent graphite carbon concentration ($C_E^{Gr} = 100\% \times (\rho_{Gr}/\rho_{Fe})$) is used during solute redistribution after graphite growth. Since the CA method for solute redistribution may introduce local solute allocation errors, the total solute amount in the domain is 统计和补偿 (statistically compensated) at each time step before calculating carbon diffusion throughout the domain. As previously described, heat extraction causes temperature decrease, while graphite and austenite precipitation releases latent heat, causing temperature increase. The combined effect on domain temperature is calculated using Equation (4). Changes in temperature and concentration fields subsequently affect graphite and austenite nucleation and growth, initiating a new cycle. Thus, this model encompasses the physical mechanism of microstructure evolution during divorced eutectic solidification of spheroidal graphite cast iron, coupling concentration and temperature field calculations with graphite and austenite nucleation, growth, and interaction processes. The physical properties of Fe-C alloys used in this work are listed in Table 1 [19].

2.1 Microstructure Evolution of Hypereutectic Spheroidal Graphite Cast Iron During Solidification

In this work, the effect of Si is considered using carbon equivalent, calculated by Equation [21] as CE = %C + 0.3%Si, to compare some simulation results with experimental data. Figure 1 [Figure 1: see original paper] shows the simulated microstructure and concentration field evolution during solidification of spheroidal graphite cast iron with an initial carbon concentration C0 = 4.71 wt% (mass fraction). The computational domain consists of 200$×$200 cells with a cell size of 2 m. To better compare with experimental micrographs, nucleation positions for some graphite nodules and austenite in the domain were artificially set for the simulation shown in Figure 1. The initial temperature is the graphite liquidus temperature of 1357 °C corresponding to the C0 composition. When the Fe melt temperature falls below the graphite liquidus temperature, graphite continuously precipitates from the liquid with decreasing temperature. When the temperature reaches the eutectic temperature Teut, austenite begins to precipitate. The heat extraction rate above (Teut - 10) °C is -4.6exp(-0.0031t), and below this temperature, the cooling rate is 1 °C/s. The temperature field is influenced by both heat extraction and latent heat release during graphite and austenite solidification. The numbers in Figure 1 represent local carbon concentrations. At the beginning of solidification, graphite nucleates and grows in the liquid as the primary phase. Graphite growth absorbs solute carbon, causing the carbon concentration in the region to decrease below the initial composition C0 = 4.71%, with the concentration around graphite being slightly lower than in regions far from graphite (Figure 1a). When the temperature decreases to the eutectic temperature, austenite nucleates. At this point, the concentration in the region approaches the eutectic composition Ceut = 4.28%, with carbon concentration in the liquid near austenite being slightly higher and that near graphite being slightly lower (Figure 1b). When graphite contacts austenite, the graphite is rapidly enveloped by austenite (Figure 1c). Subsequently, austenite gradually transforms from dendritic to globular growth, and solute carbon transports from the liquid through the austenite shell to the graphite periphery, enabling graphite to continue growing within austenite. After most graphite nodules are enveloped by austenite, the carbon concentration in the liquid gradually increases (Figures 1d-e). This occurs because austenite rejects solute carbon during growth, and the diffusion coefficient of carbon in austenite is much smaller than that in liquid. Consequently, most solute rejected by austenite enters the liquid, increasing liquid concentration. At the end of solidification, austenite shells impinge, completing solidification, with each austenite grain containing multiple graphite nodules. As temperature continues to decrease after solidification, graphite continues to grow by absorbing carbon from austenite due to non-uniform concentration in austenite, and the concentration at the graphite/austenite interface is lower than in regions far from graphite (Figure 1g). Comparing the simulation result at 740 °C (Figure 1g) with the experimental micrograph (Figure 1h) [22] demonstrates that this model can simulate spheroidal graphite cast iron microstructures that agree well with experimental observations.

Figure 2 [Figure 2: see original paper] shows the variation of solid fraction, austenite volume fraction, and graphite volume fraction with temperature during solidification. Before the eutectic temperature, graphite grows in the liquid, and the graphite volume fraction increases. At the eutectic temperature, austenite forms, and the solid fraction, austenite volume fraction, and graphite volume fraction increase rapidly, indicating that solidification is primarily completed during the eutectic stage. After the solid volume fraction reaches 100%, the graphite volume fraction continues to increase slowly while the austenite volume fraction decreases, indicating a transformation from austenite to graphite phase after solidification completion.

Table 2 compares the simulated graphite volume fraction and average radius at 740 °C (Figure 1g) with experimental results (Figure 1h) and values calculated using the lever rule from the equilibrium phase diagram. The simulated graphite fraction and average radius were measured using both program calculation and Imagetool software, while experimental values were measured using Imagetool software. The results show that the values obtained by program calculation and Imagetool measurement are very close. The simulated graphite volume fraction is slightly lower than the lever rule calculation because the lever rule is based on complete equilibrium phase transformation, whereas the CA simulation incorporates non-equilibrium kinetic factors during solidification. Conversely, the simulated values are slightly higher than experimental results because the experiment is three-dimensional, and the graphite in Figure 1h may not represent the maximum cross-section of graphite nodules, while the simulation is two-dimensional. Considering these comparisons, the simulation results are reasonable.

2.2 Interaction Mechanism Between Graphite and Austenite

To investigate the interaction and competitive growth mechanisms between graphite and austenite during solidification, this work simulated the solidification process of hypereutectic spheroidal graphite cast iron with C0 = 4.65%. Four graphite nodules and one austenite dendrite were positioned in the simulation domain of 200$×$200 cells with a cell size of 2 m. The initial temperature was the graphite liquidus temperature of 1329 °C corresponding to this composition, and cooling proceeded at 3 °C/s until the temperature reached (Teut - 10) °C, after which the temperature was held constant. Figure 3 [Figure 3: see original paper] shows the simulated evolution of graphite and austenite morphologies and the concentration field. At the beginning of solidification, when the temperature falls below the graphite liquidus temperature, graphite nucleates in the liquid. As graphite grows and absorbs solute carbon, the carbon concentration in the surrounding liquid becomes lower than in regions far from graphite. The concentration around graphite II and III is slightly lower than around graphite I (Figure 3a) because graphite II and III jointly consume solute carbon in their vicinity, resulting in lower local carbon concentration. As the temperature decreases to the eutectic temperature, austenite nucleates (Figure 3b). During austenite growth, it first envelops the nearest graphite I, then envelops graphite II and III, forming austenite shells and continuing to grow. Since austenite rejects solute carbon during growth while graphite absorbs solute carbon, the carbon concentration in regions around austenite is higher than around graphite (Figures 3b-g).

Figure 4 [Figure 4: see original paper] shows the growth velocity and radius of graphite nodules as functions of time during solidification, where growth velocity is calculated from the growth rate of the average graphite radius. At the beginning of solidification, all three graphite nodules grow at relatively high velocities. As graphite grows in the liquid and absorbs solute carbon, the carbon concentration in the liquid decreases rapidly, creating concentration gradients around graphite. According to Equation (7), the decrease in carbon concentration at the graphite interface leads to reduced graphite growth velocity, which subsequently reaches a relatively stable value (Figure 4a) because the concentration around graphite remains essentially constant (Figures 3b-d). From the beginning of solidification until 11 s, the concentration around graphite I is slightly higher than around graphite II and III (Figures 3a-c), so its growth velocity is slightly faster than the other two nodules. Subsequently, austenite begins to envelop graphite I (Figure 3d). The solute rejected during austenite growth promotes graphite I growth, significantly increasing its growth velocity. After graphite I is completely enveloped by austenite, its growth velocity rapidly decreases to below that of graphite II and approaches a relatively stable value. This occurs because graphite growing within austenite must absorb solute through the austenite shell, and the slower diffusion of carbon in austenite reduces the growth velocity of enveloped graphite I. At this moment, graphite II is still growing in the liquid, so its growth velocity is faster than graphite I. As solidification proceeds, austenite gradually approaches graphite II and III, and the growth velocity variation patterns of these two nodules during contact and interaction with austenite are similar to graphite I. When approached and enveloped by austenite, their growth velocities increase significantly, but after complete envelopment, their growth velocities rapidly decrease to relatively stable values. Figure 4b shows that at the beginning of solidification, the radii of the three graphite nodules are similar. As solidification proceeds, graphite I has a larger radius than the other two nodules, and the radius variation patterns during envelopment by austenite are similar to the growth velocity patterns. Additionally, throughout solidification, graphite III has lower growth velocity and radius than the other two nodules because it is influenced by the two surrounding graphite nodules, resulting in the smallest final size and an elliptical morphology.

2.3 Effect of Cooling Rate on Spheroidal Graphite Cast Iron Solidification

In actual solidification processes, for spheroidal graphite cast iron with a given composition, different cooling rates affect the size and size distribution of graphite nodules, thereby influencing the macroscopic properties of castings. This work simulated and analyzed the effect of cooling rate on graphite nodule size in solidification microstructures of spheroidal graphite cast iron with C0 = 4.31%. The simulation domain and cell size were the same as in Figure 3. The number of graphite nodules was determined from experimental measurements in literature [23], converted from 3D to 2D area density using the formula NA = (NV/2.37)^(2/3), where NA and NV are the numbers of graphite nodules per unit area and per unit volume, respectively. Literature [23] suggests that particles smaller than 5 m are mostly inclusions and micropores; therefore, particles in this size range were excluded when calculating graphite nodule numbers from literature [23], yielding nucleation densities of approximately 700 mm^-2 and 1400 mm^-2 for plate thicknesses of 4 mm and 1.5 mm, respectively. The number of austenite dendrites per unit area (NAg) was calculated using the nucleation model from literature [18]: NAg = 4.81$\$\times 10^{7} + 5.33\times 10^{-}6(dT/dt) + 8.7\times\$10^{4(\mathrm{dT/dt})}2$. Since literature [23] did not provide cooling rates corresponding to different plate thicknesses, the heat extraction rates in this simulation were determined from experimental values in literature [24], with heat extraction rates of 16 °C/s and 21 °C/s for plate thicknesses of 4 mm and 1.5 mm, respectively. The cooling rate in the domain is influenced by both heat extraction and latent heat release. Based on experimental observations that undercooling for graphite and austenite nucleation increases with cooling rate [24], the initial temperature for the 4 mm plate was set at the graphite liquidus temperature Tliqu corresponding to the initial composition, with primary graphite nucleating in the liquid. When the domain temperature decreased to (Teut - 15) °C, austenite nucleated. When the temperature further decreased to (Teut - 35) °C, eutectic graphite nucleated. For the 1.5 mm plate, the nucleation temperatures for primary graphite, austenite, and eutectic graphite were (Tliqu - 20) °C, (Teut - 25) °C, and (Teut - 45) °C, respectively. Nucleation positions for graphite and austenite were randomly determined.

Figures 5 [Figure 5: see original paper] and 6 [Figure 6: see original paper] show the size distribution and morphology of graphite nodules under different heat extraction rates for spheroidal graphite cast iron with C0 = 4.31%. As the cooling rate increases, the number of graphite nodules increases, the peak in the size distribution becomes more pronounced, and the peak shifts from right to left toward smaller graphite radii, with the maximum graphite diameter also decreasing. This indicates that most graphite nodule radii decrease with increasing cooling rate. At lower cooling rates, the graphite size distribution exhibits two peaks due to the two-step nucleation mechanism of primary and eutectic graphite. As cooling rate increases, the time between the two nucleation steps shortens, limiting primary graphite growth before eutectic graphite formation, resulting in a single-peak size distribution. Comparing the simulation results in Figures 5 and 6 with experimental data reported in literature [23] shows good agreement in the variation patterns of graphite size distribution and morphology with cooling rate.

To further investigate the effect of cooling rate on the average graphite nodule radius, simulations for plate thicknesses of 3 mm and 2 mm were added based on Figure 5. The calculation method for graphite and austenite numbers per unit area was the same as for Figure 5, with graphite nucleation densities of 880 mm^-2 and 1160 mm^-2 for 3 mm and 2 mm plates, respectively, and heat extraction rates of 18 °C/s and 20 °C/s. For the 3 mm plate, nucleation temperatures for primary graphite, austenite, and eutectic graphite were (Tliqu - 8) °C, (Teut - 19) °C, and (Teut - 39) °C, respectively. For the 2 mm plate, these temperatures were (Tliqu - 16) °C, (Teut - 23) °C, and (Teut - 43) °C. Other simulation conditions were the same as for Figure 5. Figure 7 [Figure 7: see original paper] shows the relationship between average graphite radius and solidification time. As solidification time shortens, the average graphite radius decreases because shorter solidification time means higher cooling rate, which produces more graphite nodules. For spheroidal graphite cast iron with a given initial composition, the final graphite volume fraction does not change significantly; therefore, higher cooling rate results in smaller final average graphite nodule radius. Figure 7 also demonstrates that simulation results are consistent with experimental results in terms of the observed trends.

Conclusions

(1) The multi-phase cellular automaton (MCA) model established in previous work was improved to simulate microstructure evolution of spheroidal graphite cast iron solidifying in a divorced eutectic manner. The model employs a local solute equilibrium approach to calculate graphite and austenite growth, using the difference between interfacial equilibrium composition and actual composition as the growth driving force. The density ratio between graphite and Fe is incorporated in the graphite growth kinetics calculation. This model can simulate divorced eutectic solidification microstructures of spheroidal graphite cast iron that agree well with experimental observations. The simulated graphite volume fraction and average radius are slightly higher than experimental measurements but slightly lower than lever rule calculations, reflecting the kinetic effects incorporated in the simulation results.

(2) The interaction and competitive growth mechanisms between graphite and austenite phases during spheroidal graphite cast iron solidification were analyzed. Results show that austenite growth in the liquid promotes the growth of nearby graphite. The growth of both phases is controlled by carbon diffusion. After graphite is enveloped by austenite, its growth velocity decreases significantly because the diffusion coefficient of carbon

in austenite is much smaller than that in liquid. Additionally, competitive growth exists among adjacent graphite nodules. Furthermore, austenite grows in a dendritic morphology before contacting graphite nodules; after enveloping graphite nodules, it grows in a globular manner, losing its original dendritic characteristics.

(3) The effect of cooling rate on graphite nodule size distribution and average radius at the end of solidification was investigated. Results indicate that at lower cooling rates, the graphite size distribution exhibits two peaks due to the two-step nucleation of primary and eutectic graphite. As cooling rate increases, the time between the two nucleation steps shortens, limiting primary graphite growth before eutectic graphite formation, resulting in a single-peak size distribution that shifts toward smaller radii. Higher cooling rate leads to shorter solidification time and smaller average graphite nodule radius. Simulation results agree well with experimental data reported in literature.

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Note: Figure translations are in progress. See original paper for figures.

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