Cellular Automaton Modeling of Microporosity Formation during Solidification of Aluminum Alloys

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A two-dimensional (2D) cellular automaton (CA)-finite difference method (FDM) model is proposed to simulate the dendrite growth and microporosity formation during solidification of aluminum alloys. The model involves a three-phase system of liquid, gas, and solid. The growth of both dendrite and gas pore is simulated using a CA approach. The diffusion of solute and hydrogen is calculated using the FDM. The model is applied to simulate the formation and interactions of dendrites and micropores in an Al-7wt.%Si alloy. The effects of initial hydrogen concentration and cooling rate on microporosity formation are investigated. It is found that the porosity nuclei with larger size grow preferentially, while the growth of the small porosity nuclei is restrained. The competitive growth between porosities and dendrites is also observed. With the increase of initial hydrogen concentration, the incubation time of porosity nucleation and growth decreases, and the percentage of porosity increases, while porosity density does not increase apparently. With the decrease of cooling rate, porosity nucleates and starts to grow at higher temperatures, and the percentage of porosity increases, but the porosity density displays a decreasing trend. In addition, at a slower cooling rate, the competitive growth between porosities and dendrites becomes more evident, leading to a more non-uniform distribution of porosity size, and an increased maximum porosity size. The simulation results agree reasonably with the experimental data in the literature.

KEY WORDS: modeling; solidification; microporosity; cellular automaton; aluminum alloys.

1. Introduction

Aluminum castings are widely used in automobile and aerospace industries and other commercial applications due to their high strength-to-weight ratio, good corrosion resistance, and relatively low raw material cost.1) However, the casting process can introduce the defect of microporosity into the components. The porosity defect reduces mechanical properties of aluminum castings such as ultimate strength, yield strength, ductility, and fatigue resistance significantly, and thus limits their applications, in particular, in critical safety components. It is commonly believed that the occurrence of the microporosity defect in castings is attributed to two concomitant mechanisms: the inadequate feeding of the volumetric shrinkage of liquid, and the insoluble hydrogen gas evolution during solidification.2,3)

Because of the fundamental and practical importance, extensive efforts have been devoted to develop models for predicting the occurrence of porosity in castings. As reviewed by Lee et al.21) and Stefanescu,3) most models,4–19) such as analytical solutions, criteria functions, Darcy’s law coupled with the conservation and continuity equations, and gas diffusion-controlled pore growth models, focus on predicting the amount of porosity in a solidified casting, but without graphical morphology output.

Researchers also developed various models that can provide direct views of the evolution of porosity formation and the interplay between gas pores and the solidified phase.20–31) Huang et al.,20) Lee et al.,21–24) and Dong et al.25) developed the cellular automaton (CA) coupled with hydrogen diffusion-controlled growth models to simulate the meso-scale morphologies of grain structure and porosity in two and three dimensions. Sasikumar et al.26) proposed a diffusion-based CA model to simulate the initiation and growth of hydrogen pores from pre-existing bubbles in a solidifying eutectic Al–Si melt. It is found that small pre-existing bubbles have a quiescent stage of very slow growth until a critical supersaturation is built up, followed by a stage of rapid growth. Because of the artificial anisotropy caused by the CA square mesh, the simulated bubbles show the non-realistic square shape. In addition, the model did not include the simulation of dendrite growth. The hydrogen for bubble growth comes in from the bottom boundary. Karagadde et al.27) adopted a new level-set (LS) approach to simulate the growth and movement of hydrogen bubbles under free growth conditions in a melt. Nevertheless, the model also could not describe the coupling growth of dendrite and porosity, either. Meidani et al.28,29) developed the two and three dimensional phase-field (PF) models to describe the non-spherical morphology of pores constrained by a solid network that consists of a symmetric array of dendrite arms.
generated in the beginning of simulations. The influence of the dendrite arm spacing (DAS) and the solid fraction on the morphology of a pore was studied. Wu et al.\textsuperscript{30} and Chen et al.\textsuperscript{31} constructed lattice Boltzmann method (LBM)-CA coupled model to simulate dendrite growth and bubble formation during solidification. The simulation results reproduce some physical phenomena, including dendritic competitive growth, the preferential nucleation locations of bubbles and bubble growth, coalescence, and motion in the liquid channels.

In the present work a CA-FDM coupled model is proposed, which includes a complete time-dependent interaction of dendrite solidification, the nucleation and growth of porosities, solute and hydrogen partitions at the interface, and the diffusion of both solute and hydrogen, to simulate the dendrite growth and microporosity formation. The model is adopted to simulate the nucleation and growth of microporosity, the interactions between dendrites and micropores, as well as the microsegregation evolution of both hydrogen and solute silicon during solidification of an Al-7wt.%Si alloy. The effects of initial hydrogen content and cooling rate on microporosity formation and morphology of a pore were studied. Wu \textit{et al.}\textsuperscript{30} and Chen \textit{et al.}\textsuperscript{31} constructed lattice Boltzmann method (LBM)-CA coupled model to simulate dendrite growth and bubble formation during solidification. The simulation results reproduce some physical phenomena, including dendritic competitive growth, the preferential nucleation locations of bubbles and bubble growth, coalescence, and motion in the liquid channels.

The emphasis of the present work is to simulate the microporosity formation due to the differences in hydrogen solubility in the solid and liquid phases, while solidification shrinkage is ignored. Hydrogen is far less soluble in solid aluminum than in liquid aluminum. During solidification of aluminum alloys, the growing dendrites reject not only solute but also hydrogen atoms into the surrounding liquid phase. When the hydrogen concentration in liquid exceeds a critical supersaturation level, the excess atomic hydrogen is separated to form gas pores. Then, the formed pores become sinks for the supersaturated gas in liquid. The growing dendrites and gas pores produce an hydrogen gradient ahead of the solid/liquid (S/L) and gas/liquid (G/L) interfaces. The growing dendrites also yield solute gradient ahead of the S/L interface. Thus, hydrogen and solute transport takes place in the domain. The effects of buoyancy, Marangoni flow, and external forces are not involved in the present model. Therefore, the formed gas porosity is stationary, and the hydrogen and solute transport is controlled by pure diffusion. In addition, the temperature in the domain is assumed to be uniform and cooled down with a cooling rate. The eutectic solidification is not considered, and the simulations are stopped when the temperature is cooled down to the eutectic temperature.

### 2. Governing Equations and Numerical Algorithm

#### 2.1. Model Description

The ratio of the local hydrogen concentration and the local saturation in liquid phase, \( S_l = C_l / S_l \), is taken as the criterion for porosity nucleation. It is assumed that the number of gas pore nuclei can be evaluated by the distribution function \( dn/dS \) that is given by

\[
\frac{dn}{dS} = \begin{cases} 
N_{\text{max}} & \left( S_{\text{max}} - S_{\text{min}} \right) \left( C_l / S_l > S_s \right) \quad (1) \\
0 & \left( C_l / S_l \leq S_s \right) 
\end{cases}
\]

where \( N_{\text{max}} \) is the maximum pore nucleation density, \( S_{\text{max}} \) and \( S_{\text{min}} \) are the maximum and minimum porosity nucleation saturation, respectively, which could be measured by experiment.\textsuperscript{10,24} \( S_s \) is the critical saturation criterion for porosity nucleation, \( C_l / S_l \) are the local hydrogen concentration (mol/m\(^3\)) and the local hydrogen saturation in liquid, respectively. When the local hydrogen saturation is satisfied with the pore nucleation condition, a pore with a certain radius is nucleated.\textsuperscript{10}

According to Sievert’s law, the hydrogen saturation in liquid, \( S_l \), of Al–Si alloys can be calculated by\textsuperscript{10}

\[
S_l = \left[ \frac{P_r}{P_{\text{ref}}} \right]^{0.6} \left[ \frac{760}{T} \right]^{0.6} \quad (2)
\]

where \( P_r \) is the internal pressure of a gas pore, \( P_{\text{ref}} \) is the reference pressure and it is taken as the standard atmospheric pressure, namely, \( P_{\text{ref}} = 1 \) atm in the present work, \( W_\text{sl} \) is the mass fraction of solute Si, and \( T \) is the temperature in the domain.

In the present work, the internal pressure of a gas pore, \( P_g \), only includes the effects of the atmospheric pressure and surface energy pressure, but the effects of the metallocstatic pressure and shrinkage pressure are neglected. Thus, \( P_g \) in the two dimensions can be calculated by

\[
P_g = P_{\text{ref}} + \lambda_{LG} / r_p \quad \text{................................. (3)}
\]

where \( \lambda_{LG} \) is the surface tension of the liquid/gas interface, and \( r_p \) is the pore radius. The radii of gas pore nuclei formed under different hydrogen saturations are also calculated using Eqs. (2) and (3).

#### 2.2. Porosity Nucleation

Pore nucleation can occur when the gas dissolved in the liquid, \( C_l / S_l \), exceeds a critical supersaturation level.\textsuperscript{3} In the present work, a stochastic model is adopted to describe porosity nucleation. The ratio of the local hydrogen concentration and the local saturation in liquid phase, \( S_l = C_l / S_l \), is taken as the criterion for porosity nucleation. It is assumed that the number of gas pore nuclei can be evaluated by the distribution function \( dn/dS \) that is given by

\[
\frac{dn}{dS} = \begin{cases} 
N_{\text{max}} & \left( S_{\text{max}} - S_{\text{min}} \right) \left( C_l / S_l > S_s \right) \quad (1) \\
0 & \left( C_l / S_l \leq S_s \right) 
\end{cases}
\]
where $V_i$ is the cell volume, and $\sum A f_g$ is the sum of gas fractions of all cells that are located at the pore $A$.

The gas inside a pore is assumed to obey the ideal gas law. Thus, the gas volume increment of the pore $A$, $\Delta V^A$, in one time step interval can be calculated by

$$\Delta V^A = R(H)^{A}_{G/L} \cdot \frac{RT}{P_g} \quad \text{................. (5)}$$

where $R(\text{H})^{A}_{G/L}$ is the quantity of hydrogen absorbed by all G/L interface cells of the pore $A$, and $R$ is the gas constant. Therefore, the gas volume increment of the G/L interface cell $(i,j)^A$ that is located at the pore $A$ can be evaluated by

$$\Delta V(i,j)^A = \Delta V^A \cdot G_s(i,j)^A \sum A G_s^A \quad \text{................. (6)}$$

where $G_s(i,j)^A$ is the geometrical factor of the G/L interface cell $(i,j)^A$, $J$ denotes all G/L interface cells of the pore $A$, and $\sum A G_s^A$ is the sum of geometrical factors of all G/L interface cells of the pore $A$. The geometrical factor $G_s$ is related to the state of neighbor cells, which is defined by

$$G_s = \min \left[ \frac{1}{2} \left( \sum_{m=1}^{4} S_m^l + \frac{1}{\sqrt{2}} \sum_{m=1}^{4} S_m^h \right) \right] \quad \text{................. (7)}$$

where $S_m^l$ and $S_m^h$ indicate the state of the nearest neighbor cells and the second-nearest neighbor cells, respectively, and $f_g$ is the gas fraction of neighbor cells. The geometrical factor defined by Eq. (7) is used to account for the effect of neighbor cell state on pore growth. Equation (7) also reflects the consideration that the geometrical relation between cells is proportional to the cell spacing, i.e., the effect of the second nearest neighbor cells is weaker than those of the nearest cells.

At one time step interval, $\Delta t$, the gas fraction increment of the G/L interface cell $(i,j)$ can be calculated by

$$\Delta f_g(i,j) = \frac{\Delta V(i,j)}{V_c} \quad \text{................. (8)}$$

Thus, at time $t_n$, the gas fraction of the G/L interface cell $(i,j)$ can be calculated by

$$f_g^{n+1}(i,j) = \sum_{n=1}^{N} \Delta V_g(i,j) \Delta t \quad \text{................. (9)}$$

where $N$ indicates the number of iterations after the cell becomes an interface cell, namely, when the cell is captured as a G/L interface cell, $N$ is set as 1. As $N$ increases, the gas fraction in this G/L interface cell increases. At the end of each time step, the gas fraction of each cell is updated according to Eq. (9). When $f_g^{n+1}(i,j) = 1$, the cell $(i,j)$ transforms its state from the G/L interface to gas pore and gets the same pore index as its gas neighbor. This newly formed gas cell in turn captures a set of its liquid neighbors to be the new G/L interface cells. The pore growth will thus continue in the next time step.

The growth of dendrites is driven by the local undercooling. The total local undercooling at the S/L interface at time $t$, $\Delta T(t)$, is given by

$$\Delta T(t) = T_i - T(t) + m \cdot (C(t) - C_0) - \Gamma(\theta) \cdot K(t) \quad \text{................. (10)}$$

where $T_i$ is the liquidus temperature, $T(t)$ and $C(t)$ are the local temperature and local solute concentration at time $t$, respectively, $m$ is the molar slope, $C_0$ is the initial composition, and $\Gamma(\theta)$ is the Gibbs-Thomson coefficient incorporated with the anisotropy of surface energy. The interface mean curvature $K(t)$ is calculated using the counting-cell method.32

The interface growth velocity, $V_g$, and local undercooling are related by the classical sharp interface model33,34

$$V_g = \mu_k(\theta) \cdot \Delta T(t) \quad \text{................. (11)}$$

where $\mu_k$ is the interface kinetics coefficient incorporated with the kinetic anisotropy.

For an fcc-lattice crystal of Al–Si alloys used in the present simulations, it exhibits a four-fold anisotropy of the kinetics and surface energy at the S/L interface.

$$\mu_k(\theta) = \bar{\mu}_k \left[ 1 + \delta_k \cos \left( 4(\theta - \theta_0) \right) \right] \quad \text{................. (12)}$$

$$\Gamma(\theta) = \Gamma_0 \left[ 1 - \delta \cos \left( 4(\theta - \theta_0) \right) \right] \quad \text{................. (13)}$$

where $\bar{\mu}_k$, $\delta_k$, $\Gamma_0$, and $\delta$ are the average interface kinetic coefficient, the degree of the kinetic anisotropy, the average Gibbs-Thomson coefficient, and the degree of the surface energy anisotropy, respectively. $\theta$ is the angle between the normal of the S/L interface and the horizontal direction, and $\theta_0$ is the preferred growth orientation of the dendrite. The angle $\theta$ can be calculated according to the gradient of solid fraction at the S/L interface using the following equation.

$$\theta = \arctan \left( \frac{\partial f_g}{\partial y} / \frac{\partial f_g}{\partial x} \right) \quad \text{................. (14)}$$

The growth velocities of the S/L interface cells are calculated by Eqs. (10)–(14). The increment of solid fraction of an interface cell at one time step could thus be evaluated from crystal growth velocity, $V_g$, as follows

$$\Delta f_s = G_s \frac{V_g}{\Delta t} \quad \text{................. (15)}$$

where $\Delta t$ is the time step, $\Delta x$ is the cell spacing, and $G_s$ is a geometrical factor related to the states of neighboring cells, defined by an equation with an identical form of Eq. (7). The only difference is that the gas fraction, $f_g$, in Eq. (7) is replaced by the solid fraction, $f_s$.

According to Eq. (15), at time $t_n$, the solid fraction of the S/L interface cell labeled as $(i,j)$ can be calculated by

$$f_s^{n+1} = \sum_{n=1}^{N} G_s^{n+1} \cdot \frac{V_g^{n+1}(i,j)}{\Delta t} \quad \text{................. (16)}$$

At the end of each time step, the solid fraction of each cell is updated according to Eq. (16). When $f_s^{n+1}(i,j) = 1$, cell $(i,j)$ transforms its state from interface to solid and gets the same crystallographic orientation index as its solid neighbor. This newly solidified cell in turn captures a set of its liquid neighbors to be the new S/L interface cells.
tion will thus continue in the next time step.

2.4. Solute and Hydrogen Transport

As dendrite grows, the solute and hydrogen partitions take place between liquid and solid at the S/L interface. On the other hand, the growing gas pores absorb the supersaturated hydrogen at the G/L interface. Thus, the solute and hydrogen gradients are yielded ahead of the S/L and G/L interfaces, leading to the solute and hydrogen diffusion. The governing equation for solute and hydrogen diffusion within the entire domain is given by

$$\frac{\partial C_i(X)}{\partial t} = D_i(X) \cdot \nabla^2 C_i(X) + R(X) \quad \cdots \cdots \quad (17)$$

where $C_i(X)$ is the concentration, $D_i(X)$ is the diffusion coefficient, $X$ is Si or H and represents solute silicon or hydrogen, the subscript $i$ is $s$ or $l$ and indicates solid or liquid, respectively. The second term on the right hand side of Eq. (17), $R(X)$, denotes the effect of solute or hydrogen partition at the interface on the concentration fields. For the solute Si concentration field, $R(Si)$ indicates the amount of solute rejected at the S/L interface. For the hydrogen concentration field calculation, $R(H)$ includes hydrogen partitions at the S/L interface, $R(H)_{S/L}$ and the G/L interface, $R(H)_{G/L}$.

When solid phase grows, the solute and hydrogen partitions between liquid and solid at the S/L interface are considered according to

$$C_i^s(X) = k_s C_i^s(X) \quad \cdots \cdots \quad (18)$$

where $k_s$, $C_i^s(X)$, and $C_i^l(X)$ are the partition coefficient and the interface concentrations of solute Si or hydrogen in solid and liquid phases, respectively. Therefore, at one time step interval, the increment of solid fraction, $\Delta \delta_s$, at the S/L interface will release the amount of solute Si, $R(Si)$, and hydrogen, $R(H)_{S/L}$, which could be evaluated by

$$R(Si) = D_i \left( C_i^s(Si) (1 - k_s) \right)$$

and

$$R(H)_{S/L} = D_i \left( C_i^l(H) (1 - k_{H,l}) \right),$$

respectively.

On the other hand, at the G/L interface, when the local hydrogen concentration, $C_i(H)$, is higher than the local hydrogen saturation in liquid, $S_l(H)$, the supersaturated hydrogen will be absorbed by the gas pore. Thus, at one time step interval, the amount of hydrogen absorbed by a pore donated as $A$ through the G/L interface cells, $R(H)_{G/L}$, could be evaluated by

$$R(H)_{G/L} = \sum_j (1 - f_i^A - f_i^S) \left( C_i^l(H) - S_i^l(H) \right) \dot{V}_e \quad \cdots \cdots \quad (19)$$

where $D_i$ denotes all G/L interface cells of the pore $A$, and $f_i^A$, $f_i^S$, $C_i^l(H)$, and $S_i^l(H)$ represent the solid fraction, gas fraction, hydrogen concentration, and hydrogen solubility in liquid, respectively, at the G/L interface cell that is located at pore $A$.

Equation (17) is solved using an explicit finite difference scheme, and the zero-flux boundary condition is adopted. The time step, $\Delta t$, is determined by

$$\Delta t = \min \left\{ \frac{\Delta x^2}{4.5 D_i(Si)} \cdot \frac{1}{4.5 \times \Delta f_{\delta_{s,max}}} \right\} \quad \cdots \cdots \quad (20)$$

where $D_i(Si)$ is the diffusion coefficient of solute Si in liquid phase, and $\Delta f_{\delta_{s,max}}$ is the maximum increment of solid fraction in one time step. Since the diffusion coefficient of hydrogen in liquid is about two orders of magnitude larger than that of solute Si, the stable time step for the hydrogen concentration field calculation is about two orders of magnitude smaller than that determined by Eq. (20).

2.5. Coupling Growth of Microporosity and Dendrite

Dendritic growth is simulated by solving the Eqs. (10)–(16). At this stage, the solid fraction increment, $\Delta \delta_s$, evaluated by Eq. (15) will give rise to the solute and hydrogen partitions around the S/L interface according Eq. (18). The rejected amount of solute Si and hydrogen, $\Delta C_i(X) = D_i \left( C_i^s(Si) (1 - k_s) \right)$ and $R(H)_{S/L} = D_i \left( C_i^l(H) (1 - k_{H,l}) \right)$, respectively.

Then, the increment of gas fraction at the G/L interface is calculated using Eqs. (2)–(8) and (19). Meanwhile, the radii of gas pores are updated by Eq. (4). This series of calculations are repeated until the end of simulation. Consequently, the physical mechanisms of a complete time-dependent interaction of dendrite growth, the nucleation and growth of porosities, solute and hydrogen partitions at the interface, and the diffusion of solute and hydrogen is embedded in the present model.

The physical property parameters used in the simulations are listed in Table 1.

3. Results and Discussion

3.1. Effect of Initial Hydrogen Concentration

The proposed model is applied to simulate gas porosity formation during solidification of an Al-7wt.%Si alloy. The calculation domain consists of a 300×300 mesh with a uniform mesh size $\Delta x=3 \mu m$. The porosity nucleation parameters used are as follows: the maximum pore nucleation density $N_{max}=1\times10^{11} \text{m}^{-2}$, the minimum and maximum pore nucleation saturations $S_{min}=1.6$ and $S_{max}=2.3$, and the critical saturation criterion $S_c=1.2$. These porosity nucleation parameters are taken as constant in all simulations in the present work. The initial hydrogen concentration is 0.55 mol/m$^3$ and the cooling rate is set to be 5°C/s. At the beginning of the simulation, several solid seeds with various crystallographic orientations are randomly assigned in the calculation domain. Figure 1 presents the evolution of porosities and dendrites of an Al-7wt.%Si alloy shown in hydrogen concentration and solute Si fields, respectively. The numbers in Figs. 1(a)–1(d) indicate the local hydrogen
concentration. It can be seen from Fig. 1 that with temperature decreasing, dendrites grow, with developing the main arms along their crystallographic orientations, and side branching of the secondary arms. The concentration of solute Si in liquid phase increases and it is obviously enriched at the S/L interface. When the temperature is cooled down to the eutectic temperature, the concentration of solute Si is increased to the eutectic composition of 12.7 wt.% Si as shown in Fig. 1(h). On the other hand, hydrogen concentration in liquid is also increased with dendrite growth, but it is less enriched at the S/L interface compared to the Si concentration. This is because the hydrogen diffusivity is about two orders of magnitude larger than the Si diffusivity. When hydrogen concentration in liquid is increased to be higher than the supersaturation for porosity nucleation, several gas pore nuclei with different radii appear when the temperature is cooled down to about 603°C as shown in Fig. 1(b). Since porosity nucleation consumes some hydrogen atoms, the hydrogen concentration in liquid is also increased with dendrite growth, leading to the growth of gas pores, as shown in Figs. 1(c) and 1(d). It is noted that some small pore nuclei nearly do not grow even when the temperature is cooled down to the eutectic temperature, although the local hydrogen concentration around the small pores is actually higher than that around the larger pores. As shown in Fig. 1(c), the local hydrogen concentration close to the two small pores, and to the two relative larger pores, is around 0.73 mol/m³ and 0.61 mol/m³, respectively. Nevertheless, the two relatively large pores are able to grow, while the two small pores cannot grow as shown in Fig. 1(d). According to Eq. (3), the internal pressure $P_g$ of a small pore is larger than that of a large pore, resulting in a larger solubility $S_l(H)$ of small pore than that of large pore (Eq. (2)). According to Eqs. (5) and (19), the larger the internal pressure $P_g$ and solubility $S_l(H)$, the smaller the gas volume increment $\Delta V$. Consequently, the growth kinetics of small pores is lower than that of large pores. Comparing Figs. 1(c) with 1(d), it also can be seen that when the temperature is decreased from 592°C to 577°C, the hydrogen concentration in liquid decreases, and the latter is even lower than the initial hydrogen concentration.

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<th>Value</th>
<th>Ref.</th>
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<td>35)</td>
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<td>36)</td>
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<td>average Gibbs-Thomson coefficient, $\Gamma$, m·K</td>
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Fig. 1. Evolution of microporosity and dendrite growth of an Al-7 wt.% Si with a cooling rate of 5°C/s and an initial hydrogen concentration of 0.55 mol/m³ at different temperatures: (a, e) 605.5°C, $F_s=15\%$, $F_g=0$; (b, f) 602.8°C, $F_s=25\%$, $F_g=0.2\%$; (c, g) 591.6°C, $F_s=48\%$, $F_g=0.578\%$; (d, h) 577°C, $F_s=53\%$, $F_g=1.426\%$; (a–d) H concentration field, (e–h) Si concentration field (Numbers in Figs. 1 (a)–1(d) show the local H concentration in liquid phase. $F_s$ and $F_g$ are the total solid fraction and percentage of porosity in the domain, respectively). (Online version in color.)
gen concentration of 0.55 mol/m$^3$. It is understandable that the growing porosities consume hydrogen atoms in liquid.

**Figure 2** shows the evolution of porosity and dendrite growth of an Al-7wt.%Si alloy with an initial hydrogen concentration of 0.65 mol/m$^3$. The other simulation conditions are identical with those of Fig. 1. It is noticed that in the early stage, the small pores grow spherically, because of the effect of the G/L interfacial tension. After the pores contact and impinge on dendrites, the growth space of pores is restricted by the complex dendrite network, and thus the pore shape becomes non-spherical. On the other hand, dendrite growth might also be impacted by the nearby pores. As shown in Figs. 2(b)–2(f), one dendritic main arm growing downwards is blocked and split by a nearby pore. Since the growing pores become sinks for the supersaturated hydrogen in liquid, the local hydrogen concentration close to pores is lower than that far away from pores as shown in Fig. 2(d). When the temperature is cooled down from around 609°C to 600°C, the overall hydrogen concentration in the domain increases as shown in Figs. 2(a)–2(d). However, when the temperature is further decreased, the hydrogen concentration decreases.  

**Figure 3** shows the solid fraction and percentage of porosity as a function of temperature with a cooling rate of 5°C/s and an initial hydrogen concentration of 0.65 mol/m$^3$.  

**Figure 4** shows the percentage of porosity varying with solidification time at a cooling rate of 2°C/s and various initial hydrogen concentrations. The other simulation conditions are identical with those of Figs. 2(a)–2(d). However, when the temperature is further decreased, the hydrogen concentration decreases, whereas pore growth rate increases. Comparing Fig. 2 with Fig. 1, it is found that with a higher initial hydrogen concentration, pore nucleation takes place at a higher temperature, and the final pore size is larger, while the porosity number does not increase evidently. This is coincidental with the experimental results obtained by James$^{37}$ and Mitrasinovic et al.$^{38}$ When the temperature is higher than about 600°C, the hydrogen concentration in liquid of Fig. 2 is higher than that in Fig. 1. However, when the temperature is cooled down to 591.6°C to 577°C, the total percentage of porosity of Fig. 2 is markedly higher than that in Fig. 1. It is evident that the higher percentage of porosity consumes more atomic hydrogen, leading to a lower hydrogen concentration in liquid, even though the initial hydrogen concentration of Fig. 2 is higher than that of Fig. 1.
tions are identical with those of Fig. 1. As shown, the general trend of the profiles in Fig. 4 is that at the early stage, the rate of porosity percentage is slow, and then increases rapidly, but at the late stage, it slows down again. In the initial stage of solidification, the percentage of porosity is zero, indicating that there is an incubation time for porosity nucleation. With the increase of initial hydrogen concentration, the incubation time of porosity nucleation decreases. This is because the increased initial hydrogen concentration leads to a higher local hydrogen concentration in liquid, and thus the hydrogen supersaturation condition for porosity formation could be satisfied sooner (see Eq. (1)). It also can be noted from Fig. 4 that the percentage of porosity increases with the initial hydrogen concentration.

3.2. Effect of Cooling Rate

Figure 5 presents the simulated hydrogen concentration field and morphologies of dendrite and microporosity when the temperature is cooled down to the eutectic temperature with different cooling rates of 2°C/s and 15°C/s. The initial hydrogen concentration is 0.5 mol/m^3. The other simulation conditions are identical with those of Fig. 1. It can be seen that with increase of cooling rate, dendrites become finer, porosity size is smaller and more uniform, but the density of porosity increases. These results are coincident with those observed experimentally. It is understandable that at a faster cooling rate, dendrites develop rapidly with finer and longer arms and side branches, so that the complex dendrite network could be formed sooner. The formed dendrite network blocks hydrogen diffusion in liquid, and thus inhibits the growth of porosities. In addition, cooling rate also influences the time for hydrogen diffusion and pore growth. A lower cooling rate will provide more sufficient time for hydrogen diffusion and pore growth, leading to the increase in pore size. Moreover, it is noted that with increase of cooling rate, the hydrogen concentration in liquid at the eutectic temperature is higher due to the fact that the percentage of porosity obtained from the faster cooling rate is lower than that from the slower cooling rate.

Figure 6 shows the percentage of porosity as a function of temperature with different cooling rates. The initial hydrogen concentration is 0.55 mol/m^3. The other simulation conditions are identical with those of Fig. 1. It can be seen that with increase of cooling rate, pores nucleate and start to grow at lower temperatures. The profile descends and the final percentage of porosity at the eutectic temperature decreases with the increase of cooling rate. The simulation results of Fig. 6 show the same trend with the experimental data obtained by Lee and Hunt. It is known that the porosity with larger size will have important impact on the fatigue strength and tensile strength. Figure 7 presents the maximum porosity radius varying with cooling rate at different initial hydrogen concentrations. Note that with the decrease of cooling rate, the final maximum porosity radius increases. In particular, when the cooling rate is reduced from 2°C/s to 0.5°C/s, the maximum porosity radius increases evidently. It is found that at a slow cooling rate, the porosity size is not uniform. The pore nuclei with relative larger size could grow to be the porosities with large size, while the small pore nuclei might not be able to grow as shown in Fig. 5(a). This is because a slow cooling rate provides longer time for the competitive growth of pores with different sizes. As discussed previously, the pore nuclei with larger size have the priority to be sinks of hydrogen in liquid, resulting in larger final porosity sizes. The total hydrogen amount in the domain is limited. In the case of a slow cooling rate, the growth condition of pore nuclei with small size might not be able to be satisfied till the end of solidification due to the fact that most of hydrogen atoms are exhausted by the growing large pores. Accordingly, with the decrease of cooling rate, the effect of the competitive growth among pores.
becomes more evident, leading to a non-uniform distribution of pore size (Fig. 5(a)) and the increased maximum porosity size as shown in Fig. 7.

4. Conclusions

A 2D CA-FDM model is proposed to simulate dendrite and porosity formation during solidification of aluminum alloys. The model involves the nucleation and growth of dendrite and porosity, the redistribution and diffusion of solute and hydrogen, and the effect of surface tension.

The model is applied to simulate the porosity formation during solidification of an Al-7wt.%Si alloy. The simulations reveal the coupling and competitive growth of dendrites and porosities, as well as the microsegregation of solute and hydrogen. It is found that with the increase of initial hydrogen concentration, the percentage of porosity increases, and the incubation time of porosity nucleation and growth decreases, while the porosity density does not increase obviously. With cooling rate decreasing, the percentage of porosity and maximum porosity radius increase. In addition, porosity nucleates and starts to grow at higher temperatures, while the porosity density shows a decreasing trend with the decrease of cooling rate.

The competitive growth between different porosities and dendrites is observed. The porosity nuclei with larger size are able to grow preferentially, while the growth of the small porosity nuclei is inhibited. Because of the effect of gas-liquid interfacial tension, the gas pore grows spherically when it is enveloped by liquid. After touching with dendrites, the growth space of porosity is restricted by the complex dendrite network, and thus becomes a complex non-spherical shape. On the other hand, the growth of dendrite might also be influenced by the nearby porosity. With cooling rate decreasing, the competitive growth between porosities and dendrites becomes more evident, leading to non-uniform porosity size, and increased maximum porosity size. The simulation results are compared reasonably well with the experimental data.

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