Three-dimensional numerical simulation of solidification microporosity and microstructure of aluminum alloys

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Abstract. A three-dimensional model was developed to study microporosity evolution with grain growth during solidification by cellular automaton method. The simulations are able to show the evolution and morphology of both grain structure and porosity. The effects of shrinkage pressure and initial hydrogen content on porosity evolution and final porosity percentage are modeled and related to the location-specific microstructure of the solidified products. A wedge die casting, providing samples of different cooling rates, was used to validate the simulation results. X-ray micro-tomography was performed to obtain the relevant porosity information. The simulated porosity size, percentage and distribution considering both shrinkage pressure and hydrogen content were found to agree well with those from experimental measurements.

1. Introduction
Aluminum alloys have been widely used in industrial applications due to the good mechanical properties of high strength-to-weight ratio, good corrosion resistance, and so on. However, porosity exists in castings known to reduce mechanical properties of casting products, in particular ultimate strength and fatigue resistance. Porosity observed in aluminum castings can be mainly divided into shrinkage porosity and gas porosity [1, 2]. Experiments have been used to investigate porosity of casting products under different processing parameters, but it is still hard to observe the porosity nucleation and evolution during solidification process and predict porosity in castings. Modeling and simulation of porosity formation [3, 4] can be used on the mechanisms of porosity formation for casting design and process optimization.

However, most of the relevant researches are only able to provide the predicted porosity level in solidification products, and there is little study on the prediction of porosity information such as distribution and size with graphical grain and porosity morphology [1]. The prediction of porosity coupled with grain of alloys is an essential part of microstructure to mechanical property predictions in integrated computational materials engineering (ICME) [5]. The understanding of the mechanism of morphological changes of grain and porosity is helpful for the porosity control in casting products, which also provides a critical link in ICME for the casting industry.

In this study, a numerical model was proposed to predict microporosity evolution during the solidification process by cellular automaton method. Both the effects of shrinkage pressure and the hydrogen content are considered in the model, which means the predicted porosity is developed by both the solidification shrinkage and the dissolved hydrogen. The evolution of porosity with multi-grains was simulated, and the porosity morphology, porosity distribution and size were obtained. The simulated results were validated with wedge die casting experiments.
2. Model description

2.1. Grain growth model
The continuous nucleation distribution [6] is used [7] for the nucleation of grains during solidification. Following nucleation, solute distribution including solute partitioning and diffusion can be calculated by:

\[ C_i^{S*} = k_iC_i^{L*} \]  \hspace{1cm} (1)

\[ \frac{\partial C_i^L}{\partial t} = \nabla \cdot (\sum_j D_{ij} \nabla C_i^L + (C_i^{L*} - C_i^{S*}) \frac{\partial f_s}{\partial t} + D \nabla ^2 C_i^L) \]  \hspace{1cm} (2)

where \( C_i^{S*} \) and \( C_i^{L*} \) are the interface solute concentrations of the solute element \( i \) in solid and liquid respectively, \( k_i \) is the solute partition coefficient, and \( D \) is the diffusion coefficient. The interface solute concentration can be calculated by [7,8]:

\[ \sum_{i} n^{-1} \frac{\partial T}{\partial C_i^{L*}} (C_i^0 - C_i^{L*}) = T_0 - T^* - \Gamma \kappa \]  \hspace{1cm} (3)

where \( T_0 \approx T_P - \sum n^{-1} \frac{\partial T}{\partial C_i^{L*}} C_i^0 \) is the liquidus temperature, \( T^* \) is the local temperature, \( \Gamma \) is the Gibbs–Thomson coefficient, and \( \kappa \) is the interface curvature. To trace the interface, the solid fraction increment can be calculated based on the lever rule [7, 8].

2.2. Porosity evolution model
In this study, pore nucleation was considered by using the stochastic porosity nucleation model [9]. Based on Sievert's law, the hydrogen saturation can be calculated by [10]:

\[ S_i^{LH} = \left( \frac{P_i}{P_o} \right)^{10^{rac{2760}{T} + 2.796 - \frac{0.0119c_i^L + 0.017c_i^M}{T}}} \]  \hspace{1cm} (4)

where \( P_i = P_0 + 2r_P - P_s \) is the pore internal pressure, \( P_0 \) is the standard atmospheric pressure, \( \gamma \) is the surface tension, \( r_P \) is the pore radius, \( P_s \) is the shrinkage pressure.

During solidification, the hydrogen content in the liquid is increased. Meanwhile, the supersaturated hydrogen in the liquid is absorbed by adjacent nucleated pores, resulting in the growth of the pore. The pore volume increment can be calculated by considering all the hydrogen absorbed:

\[ \Delta V = \frac{P_o}{P_i} V_G = \frac{P_0}{P_i} \sum_A (1 - f_S - f_G) V_{cell} \rho (C_i^L - S_i^{LH}) \]  \hspace{1cm} (5)

where \( V_{cell} \) is the cell volume, and \( \rho \) is the liquid density. According to the equations above, pore growth can be calculated considering the effects of both shrinkage pressure and hydrogen content. Thus, the evolution of microporosity and microstructure during solidification is obtained. It should be mentioned that the eutectic solidification and the effect of fluid flow are ignored in this paper.

3. Model verification
A V-shaped wedge casting experiment was developed to provide validation for simulations. Al alloy A356, was used in the experiment. Figure 1 shows the schematic geometry and the cast sample of the proposed wedge die casting. With different wall thickness, the casting experiment is able to obtain different cooling rates from top to bottom. At first, the Al ingots were melted to about 700 °C, and the melt were kept at the temperature for 30 min. During pouring, K-type thermocouples were used to simultaneously measure the corresponding temperature profiles at the three locations A, B, and C. Since instant cooling rates were used in the simulations, the instant cooling rates were calculated at the liquidus temperature from the experiment cooling curves, which were 64.8, 10.7, and 2.5 K/s at point A, B, and C, respectively.
Reduced pressure test (RPT) [11] was performed to measure the equivalently initial hydrogen which was obtained as $C_H^0 = 0.3 \text{ mL/100g Al}$. In addition, X-ray micro computed tomography (XMCT) was used to characterize the porosity information, including porosity morphology, percentage, and location of each pore. The samples were scanned at 90 kV, 80 μA and a resolution of 6.318 μm per voxel using HeliScan™ microCT.

4. Results and discussion

4.1. Grain structure and porosity simulation

Based on the proposed 3D CA model, the evolution of grain as well as porosity of Al-7Si-0.3Mg ternary alloy can be simulated as shown in figure 2. In the simulation, the calculation domain was set as a $1000 \times 1000 \times 100 \mu m^3$, and the cell size was 5 μm. A constant cooling rate of 10 K/s was adopted. The initial hydrogen concentration was 0.5 mL/100g Al, and the shrinkage pressure was 0. From the simulation result, the structures of grain and porosity are connected closely with each other. During the solidification, since the pores are encompassed by solidified grains, it is difficult for the pores to run away from the liquid and eventually result in porosity. From solute distributions of Si and Mg, the solute concentration is increased as temperature decreases due to solute partitioning. The distributions of Si and Mg are not influenced by the pores. Si and Mg concentrations in the remaining liquid are increased to their eutectic concentrations when the temperature decreases to the eutectic temperature. However, the hydrogen distribution shows much difference from the solute distributions. The hydrogen concentration shows to increase first due to hydrogen partitioning as well. As solidification proceeds, temperature continues decreasing and hydrogen content in the liquid continues increasing. When the hydrogen concentration is larger than the hydrogen saturation, the pore nucleation will happen as the nucleation criterion is fulfilled. The nucleated pores then start to grow by absorbing the adjacent saturated hydrogen, decreasing the local hydrogen concentration. Thus, hydrogen concentration decreases in the latter stages of solidification. It should be noted that with the change of temperature and local Si and Mg concentrations, local hydrogen saturation will also change, leading to the pore growth. It can be seen in the simulations that the nucleated pore continues absorbing the surrounded hydrogen. Since the diffusivity of hydrogen is much larger than that of solute, there is no obvious hydrogen gradient in the remaining liquid.

![Figure 1](image_url). Schematic geometry (a) and (b), sample (c), and cross-section (d) of wedge die casting.
Simulation results of (a) grain and porosity, (b) Si distribution, (c) Mg distribution, and (d) hydrogen distribution at different times: (a1, b1, c1, d1) 1.5 s; (a2, b2, c2, d2) 3.0 s; (a3, b3, c3, d3) 4.5 s.

Porosity percentage as a function of temperature and time with (a) shrinkage pressure of 0, 0.5, 1.0, and 1.5 atm, and (b) initial hydrogen concentrations of 0.5, 0.55, and 0.6 mL/100g Al.
Figure 3 plots the porosity percentage vs. temperature under the effect of shrinkage pressures and initial hydrogen concentrations. The simulations were performed on Al-7Si binary alloy and in a calculation domain of $500 \times 500 \times 500 \, \mu m^3$, and the cooling rates were 50 K/s. It should be noted that the porosity percentage increases with increasing shrinkage pressure, while the porosity nucleation is not influenced by the increase of shrinkage pressure in this study. It is because the porosity formation during eutectic at the end of solidification is not considered in this paper. Meanwhile, increasing initial hydrogen concentration will increase the porosity percentage. It shows that pores start to nucleate at a higher temperature with a higher initial hydrogen concentration, which is due to that higher initial hydrogen concentration will lead to more hydrogen enrichment and thus higher levels hydrogen will satisfy the nucleation criterion earlier, and the nucleation of porosity will occur more rapidly and at higher temperatures. When the initial hydrogen concentration is at a lower value, it will take more time for the local hydrogen concentration to be large enough and thus the nucleation occurs at lower temperature.

4.2. Experimental validation

As a validation with the experiments, 3D CA simulations with same condition were performed. The whole calculation domain was $1 \, mm \times 1 \, mm \times 1 \, mm$ which is the same with the microCT measurements as shown in figure 4. In the real casting, the volume change during solidification, $\Delta V_{c, w}$, can be calculated by:

$$\Delta V_{c, w} = \left(1 - \frac{\rho_l}{\rho_s}\right) V_{0, w} f_{s, w}$$

(6)

where $\rho_l$ and $\rho_s$ are the liquid density and solid density, $V_{0, w}$ is the casting volume, and $f_{s, w}$ is the solid fraction. The shrinkage pressure, $P_s$, is calculated by:

$$P_0 V_{0, w} (1 - f_{s, w}) = (P_0 - P_s) [V_{0, w} (1 - f_{s, w}) + \Delta V_{c, w}]$$

(7)

$$P_s = P_0 \left(1 - \frac{1 - f_{s, w}}{1 - \frac{P_l}{P_s}}\right)$$

(8)

As shown in microCT measurements in figure 4(a), (d) and (g), the pores show different morphologies due to the constraint of the surrounded dendrites. With decreasing cooling rate, the pore number decreases while the pores appear to have much larger sizes. Figure 4(b), (e), and (h) show the simulated porosity with transparent dendrites at the end of solidification. In the simulated results, as cooling rate decreasing, the porosity size increases and the pore number decreased as expected.

In order to clearly observe the morphology of dendrites and pores, 2-D optical microstructure with different cooling rates was measured and compared with the 2-D simulated results as shown in figure 5. The simulations and optical microstructure clearly show the porosity and dendrite morphologies. The simulated dendrite morphologies match well with the experiments as shown in figure 5(c) and (d). It should be noted that at the end of solidification, the remaining liquid will transform to eutectic as shown in both simulation and experiment. As the cooling rate decreased, the pores appear to be larger, while the morphologies of the pores are not shown to be round shape. It is because that 2-D optical microstructure is only able to provide a slice of complete 3D information [12, 13]. Even so, the 2-D simulated results of both the dendrite and porosity morphology agree well with the experiments.

Figure 6 shows the relationship between porosity percentage and cooling rate. Increasing cooling rate decreases the porosity percentage. By coupling both hydrogen and shrinkage, the simulation results show well agreement with the wedge casting experiments. It should be pointed out that the simulated results considering only hydrogen are lower than the experimental results compared to that considering both hydrogen and shrinkage. Porosity morphologies in figures 4 and 5 also point out this difference. It is because that micro-shrinkage increases the final percentage of porosity. It can be seen that the evolution of microporosity and microstructure can be predicted by using present model. The validation of the model provides an excellent opportunity for the prediction of location-specific microstructure which is helpful and essential for the casting design optimization. This microporosity and microstructure...
model shows to be a critical link between process parameters and mechanical properties in ICME researches of casting products.

![Figure 4. Porosity morphology of microCT measurements as a comparison with CA simulations: microCT (a), (d), and (g); simulated porosity (b), (e), and (h); simulated dendrite (c), (f), and (i). The cooling rates: (a)-(c) 64.8 K/s; (d)-(f) 10.7 K/s; and (g)-(i) 2.5 K/s.](image)

![Figure 5. Optical microstructure at cooling rate of: (a) 64.8 K/s, (c) 10.7 K/s, and (e) 2.5 K/s; and simulated results: (b) 64.8 K/s, (d) 10.7 K/s, and (f) 2.5 K/s.](image)
5. Conclusions
In this study, a numerical model was developed for the prediction of evolution of microporosity and microstructure during solidification of Al-7Si-0.3Mg ternary and Al-7Si binary alloys. By adopting the present model, the morphology and distribution of microporosity and microstructure can be simulated, and porosity percentage can be calculated. The effect of initial conditions were investigated. With initial hydrogen concentration increases, porosity percentage increases. In this study with high hydrogen content and pore nucleates before shrinkage occurs, with increasing shrinkage pressure the porosity percentage increases. The simulated porosity percentage and the pore distribution considering both shrinkage pressure and hydrogen content show well agreement with the experiments. The proposed 3D CA model provides an essential link between process parameters and location-specific mechanical properties for further ICME researches.

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