

Modeling of Semisolid Structure Formation in Controlled Nucleation Method

X. Yao^{1,3)} and H. Wang²⁾

1) School of Engineering, James Cook University, Townsville, QLD 4811, Australia

2) School of Engineering, The University of Queensland, St Lucia, QLD 4072, Australia

3) School of Mechanical and Electrical Engineering, East China Jiaotong University, Nanchang, China

Modeling the semisolid structure formation is of significance in both understanding the mechanisms of the formation of such structure and optimization the solidification conditions for the required structure. A modified cellular automaton (mCA) model has been developed, which is coupled with macroscopic models for heat transfer calculation and microscopic models for nucleation and grain growth. The mCA model is applied to Al-Si alloys, one of the most widely used semisolid alloys. It predicts microstructure morphology and grain size during semi-solid solidification, and determines the effects of poring temperature and mould temperature on the final microstructure. The simulated results are compared with those obtained experimentally. The resulting simulations give some insight into the mechanisms about the semisolid structure formation in Controlled Nucleation process.

KEY WORDS: Microstructure modeling, semisolid metal processing, semisolid structure formation, Al-Si alloy.

1. Introduction

Semisolid processing requires special feedstock materials with non-dendritic grain structure^[1-3]. Controlled Nucleation Method (CNM) has been approved as an effective method to produce such semisolid structure^[4, 5]. It uses solidification conditions rather than mechanical or electromagnetic stirring to control nucleation, nuclei survival and grain growth, and then achieves a fine-grained and non-dendritic microstructure for semisolid casting.

In CNM process, the main principle is to maximise grain density in the melt and promote grain growth in a non- or less-dendritic motion. The grain density again depends two factors: nucleation and nuclei survival. For nucleation, adding grain refiner is one of the common methods to provide more heterogenous particles or/and make the heterogenous nucleation more favourable. Another important source is wall crystals that can be further exploited. They are the crystals that are nucleated during pouring, at or near the relatively cold mould wall. The wall crystals are then transported to bulk melt and serve as very effective nuclei. Solidification conditions, such as pouring temperature (melt superheat), mould preheat temperature, cooling rate and thermal properties of the mould material, are the factors that influence the wall crystal formation, survival and growth, which then also affect the further nucleation of crystal in the remaining melt.

The recent progress in the simulation of microstructure formation during solidification makes it possible to predict the semisolid structure formation in CNM process [6]. A modified Cellular Automaton (mCA) has been developed by Yao [7] and others [8,9], which takes account of thermal, solute and capillary effects into nucleation and growth to simulate microstructure formation.

In this paper we investigate the effect of pouring temperature, mould preheat temperature and alloy composition on nucleation, growth, and final grain size as well, by using the mCA model. The contribution of the

wall crystal mechanism to nucleation and semisolid structure formation in CNM process has also been investigated.

2. Model descriptions

In order to verify present experimental data, modelling of semisolid structure formation has been performed under the same governing solidification conditions as used in experiments^[3]. Neglecting the effect of convection, the solidification process is controlled by thermal and solute diffusion. The equations that describe the physics of these processes are:

- Thermal diffusion:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla(\lambda \nabla T) + \rho H \frac{\partial f_s}{\partial t} \quad (1)$$

where T is temperature, t is time, λ is the thermal conductivity, ρ is the density, c_p is the specific heat and H is the latent heat.

- Solute diffusion

$$\frac{\partial C_i}{\partial t} = \nabla(D_i \nabla C_i) \quad (2)$$

where D is the interdiffusion coefficient, $i = L, S$ represent the liquid and solid phase respectively.

- Nucleation

A continuous nucleation model with Gaussian distribution^[10] was used to describe the grain density increase, dn , which is induced by an increase in the undercooling, $d(\Delta T)$. Then the total density of grains, $n(\Delta T)$, which has been nucleated at a given undercooling, ΔT , is given by

$$n(\Delta T) = \int_0^{\Delta T} \frac{dn}{d(\Delta T)} d(\Delta T) \quad (3)$$

- Growth

If the kinetics and curvature contributions of undercooling are neglected, the local undercooling at time t , $\Delta T(t)$, can be given by

$$\Delta T(t) = T^{EQ} - T(t) = T_L + m_L(C(t) - C_0) - T(t) \quad (4)$$

where T^{EQ} is the local equilibrium liquidus temperature at a local composition $C(t)$ in the liquid, T_L is the equilibrium liquidus temperature with concentration C_0 , m_L is the slope of liquidus and C_0 is the initial concentration of the alloy. Considering constitutional undercooling, the effect of solute build up is to decrease the local equilibrium liquidus temperature through the term $m_L(C(t) - C_0)$, and thus the value of undercooling is not increased. The growth velocity, $V(t)$, can be calculated using models such as the KGT model^[11].

- Interface retardation

In columnar growth, a barrier is being established by solute build-up that retards the velocity by $V_b(t)$ ^[12].

$$V_b(t) = -\frac{m_L}{G} \frac{dC_L^*}{dt} \quad (5)$$

where G is the thermal gradient at the interface. Thus, the interface advancing velocity, $V_i(t)$, is given by

$$V_i(t) = V(t) - V_b(t) \quad (6)$$

As in previous models^[10], the growth length of the dendrite tip, $L(t)$, during one time step, δt , is given by

$$L(t) = \frac{V_{real}(t) \cdot \delta t}{(\cos \theta + |\sin \theta|)} \quad (7)$$

where θ is the angle of the preferential growth direction with respect to the horizontal direction of the cell.

3. Results and Discussion

Thermophysical properties of the alloys used in the simulations are presented in Table 1.

Table 1 Thermophysical properties of Al-Si alloys^[13]

T_m^{Al} (K)	T_{eut} (K)	C_{eut} (wt%)
933	850	10.77
ρ (kg/m ³)	C_p (J/kg K)	λ (W/m K)
2720	1086	192.5
k_0 (-)	m_L (°C/%)	ΔH_V (J/m ³)
0.117	6.5	1.107×10^9
D_l (m ² /s)	D_s (m ² /s)	Γ (K m)
3×10^{-9}	1×10^{-12}	0.9×10^{-7}

3.1 Effect of pouring and mould preheat temperatures

The effect of mould preheat temperature on microstructures is shown in Figure 1 and 2 for Al-1%Si and Al-6%Si alloys, respectively, at pouring temperature 660°C. Figure 1 shows that at preheat mould temperature lower than 300°C, the domain solidified as equiaxed crystals, and the grain size increases slightly in an increase preheat mould temperature. When the temperature is above 300°C, a sudden change of the growth mode from equiaxed to columnar occurs. Increasing mould preheat temperature decreases the cooling rate to approach a smaller bulk undercooling.



Figure 1. Effect of mould preheat temperature on microstructure formation in Al-1%Si alloy, T=25, 100, 300, 350, 400, 500 °C

This undercooling decides the nucleation in the bulk liquid. It seems that the undercooling approaches a critical value when the preheat temperature is at about 300°C. Above the temperature, the bulk undercooling can only activate a very small number of particles to form equiaxed crystals, thus the castings have a tendency to form columnar crystals. For Al-6%Si alloy, figure 2 shows that even at higher preheat temperature, the domain solidified as equiaxed and the grain size remains small difference. Higher solute enrichment should enhance the extent of constitutional undercooling and restrict the growth of columnar crystals, thus it is beneficial for formation of equiaxed crystals. Lower temperature gradient is also a positive factor to CET.

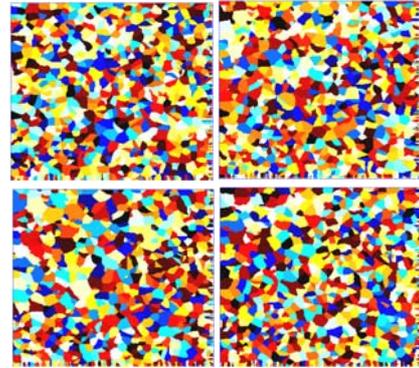


Figure 2. Effect of mould preheat temperature on microstructure formation in Al-6%Si alloy, T= 300, 350, 450, 500 °C

Increasing pouring temperature should reduce the number of the wall crystals generated at the mould walls, the subsequent survival rate of the crystals, and the temperature gradient in the liquid as well. A possible reason is that forming wall crystals needs very small undercooling, then the number of wall crystals which form at the mould walls remains relatively constant and independent to the preheat mould temperature. The wall crystals subsequently have been transported to distribute in the melt by fluid flow, and the survival of these crystals in the liquid should be only depended on the temperature of the bulk melt and the exposure time which are mainly influenced by pouring temperature and the rate of heat transfer.

Figure 3 and 4 show the effect of pouring temperature on microstructure formation for Al-6%Si alloy. The pouring temperatures were 620°C and 650°C respectively. It is reasonable to consider that the number



Figure.3. Microstructure formation and evolution in Al-6%Si alloy at a pouring temperature of 620°C. $t=100, 150$ and $300s$, calculation domain: $1mm \times 1mm$

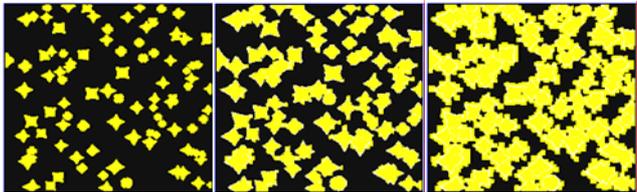


Figure 4. Microstructure formation and evolution in Al-6%Si alloy at a pouring temperature of 650°C. $t=200, 300$ and $330s$, calculation domain: $1mm \times 1mm$

of wall crystals transported by fluid flow from the mould walls in the melt is much larger than that with high pouring temperatures. In this situation, the crystals do not need an undercooling for nucleation, thus are controlled by free growth dependent on the curvature undercooling. The crystals grow in a relatively small undercooling (big enough for growth but insufficient for further nucleation of particles existed in the bulk) caused by extraction of heat to the surroundings. The large amounts of latent heat results in the recalescence to reduce the bulk undercooling, thus the particles can not be activated as nucleation sites. It should be obtained that the grain refinement of semi-solid casting with low pouring temperatures has less significant effect of that in normal solidification process.

3.2 Nucleation mechanisms

A set of experiments has been performed with gauze to investigate which the nucleation mechanism is the predominant factor to control the solidification in different pouring conditions. By creating a barrier of the flow of crystals from the walls to the centre of the casting, gauze experiments with three pouring methods are designed to isolate, enhance and balance the contributions to microstructure formation of wall crystals. In present calculation, Assumptions are given by: (1) an average undercooling, $\Delta T_{v,max} = 0.5K$, for free growth of the wall crystals; (2) no wall crystals inside gauze with pouring method I, and densities of the wall crystals inside and outside the gauze are equal both in pouring method II and III, but at different values of $n_s=5.5 \times 10^{10}$ and $n_s=1.1 \times 10^{11}$, respectively; (3) Only the wall crystals could be activated if existed.

As shown in Figure 5, in method I of pouring (only inside the gauze), transportation of wall crystals to the centre is isolated, thus microstructure formation and growth within the gauze are only depended on the constitutional undercooling that is determined by alloy composition and cooling rate. Compared with the feature of microstructure formation outside the gauze, less amount of nucleation sites and larger critical nucleation undercooling result in much larger grain size within gauze. On the other hand, in the method III of pouring (between gauze and the mould), a huge number of wall

crystals will be created by crystal fracture and crystal remelting. These wall crystals are easily carried to the centre of gauze by fluid flow to form equiaxed crystals. Therefore, the grain size within the gauze is decreased dramatically. The grain size within the gauze is a slightly larger than that between gauze and the mould because a relatively high temperature lasts longer time to eliminate some of the wall crystals by remelting. In the method of pouring both inside and outside the gauze (method II), conditions for microstructure formation are between the former two methods. Figure 6 shows comparison between prediction and experimental results.

5. Conclusions

Pouring temperature affects the survival of the “wall crystals” brought into the bulk liquid by fluid flow. High temperature pouring temperature results in a coarse grain structure. At a given temperature which allows some of the “wall crystal survival, the microstructure morphology and grain size are relatively dependent on the mould preheat temperature. Below a temperature of 300°C, a fine equiaxed grain structure is obtained and the grain size increases with the mould preheat temperature very gradually. However, a columnar growth is predominant when the temperature exceeds 300°C.

Modeling of gauze experiments shows that the grain size is dependent on the pouring method. Pouring between the mould and the gauze leads to large number of “wall crystals” existed in the bulk. If the pouring temperature is not too high to allow the crystals surviving, a very fine equiaxed grain structure is gained. Pouring in the centre of the gauze leads to elimination of “wall crystals” in the centre of the casting, which results in a large grain size, but the grains still are fine between the mould and the gauze because of the existence of the “wall crystals”. It is concluded that the mechanism of “wall crystals” is important for grain formation especially with low pouring and mould preheating temperatures, i.e. semisolid structure formation.

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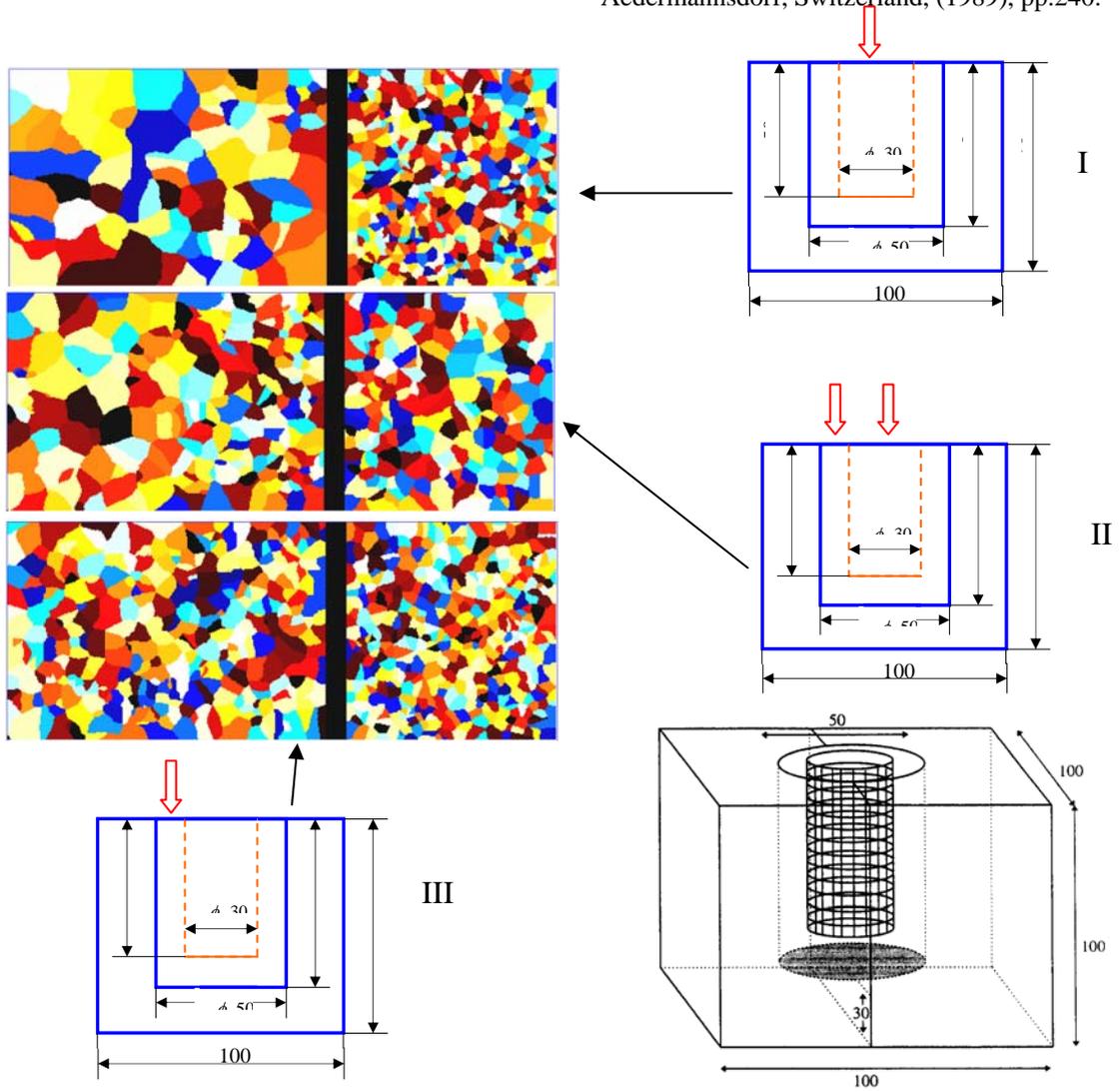


Figure 5. Effect of pouring method on microstructure formation in Al-7%Si alloy

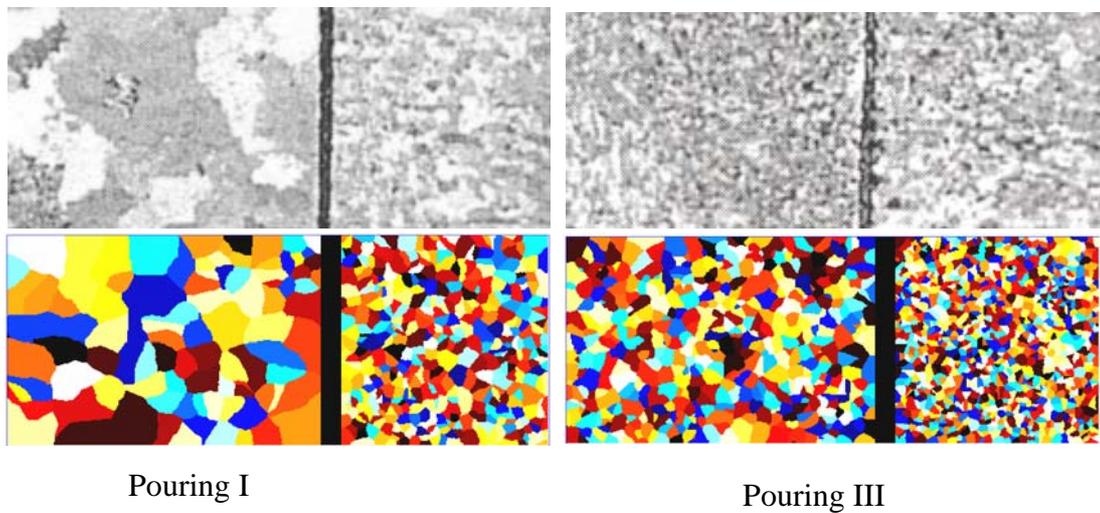


Figure 6. Effect of different pouring methods on microstructure and compared with experimental results.