Numerical Simulation of Microstructure of Al–Si/SiC\textsubscript{p} Composites during Stir Casting Process with Particle Pushing Model

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(Received on August 22, 2005; accepted on November 7, 2005)

Particle distribution has vital influence on the microstructure and the final performance of particle reinforced metal matrix composite. The formation of microstructure of SiC particle reinforced Al–7.0 mass%Si composite made by stir casting was simulated in this paper. Two-dimensional models under normal solidification condition including macro heat transfer, micro nucleation, equiaxed dendrite growth and particle pushing were presented. Two sets of meshes were used to carry out macro and micro calculation, respectively. A modified cellular automaton method coupled with finite difference method was used to simulate the evolution of the composite microstructure. In addition, the effects of SiC particle volume fraction, different casting processes, pouring temperature and cooling rate on the composite microstructure and the particles distribution were analyzed. The simulated results can clearly show the particle clustering/accumulation phenomenon caused by particle pushing. The calculated cooling curve and final predicted microstructure are in good agreement with the experimental results. Grain size is smaller for metal mould casting than sand mould casting. With the increase of SiC particle volume fraction or cooling rate, the grains of the matrix alloy are refined and particles are distributed more uniformly. As the pouring temperature increases, particles are distributed more uniformly.

KEY WORDS: metal matrix composite; particle pushing; microstructure; numerical simulation.

1. Introduction

Particle reinforced metal matrix composites (PRMMCs) have got promising development in recent years due to higher specific strength, excellent wear resistance, superior high-temperature performance and good applicability for net shape machining, which make them be successfully applied in automobiles, aeronautical/aerospace parts, sports apparatus and so on. PRMMCs may be produced by stir casting on a large scale which needs low cost and simple technology.

Solidification process of PRMMCs has vital influence on their final microstructures and mechanical properties. The process includes many complex phenomena such as heat transfer, fluid flow, solute segregation, chemical reaction, particle clustering and interface pushing, so it has many advantages to analyze and study above problems by numerical simulation. Many studies have shown that inhomogeneity of particle distribution is a key factor to the decrease of ductility and fracture toughness. In addition, particle clustering may cause other deleterious effects such as local stress concentration, residual stress increase and porosity formation. Inhomogeneity of particle distribution caused by particle clustering is related to the fact that particles are pushed by solidification interface. So it is the key of numerical simulation to accurately predict particle pushing/engulfment phenomena and particle final distribution.

Previous numerical modeling studies on solidification process of PRMMCs mainly focused at macroscopic scale. Rohatgi \textit{et al.}\textsuperscript{3} presented a simple one-dimensional model based on solidification experiment and studied the effect of stationary particle on temperature profiles and interface velocities. Beckermann \textit{et al.}\textsuperscript{4,5} presented a multiphase model based on the volume-averaged technology and predicted the macroscopic particle distribution and the advancing speed of solidification front. Previous particle distribution simulation at microscopic scale mainly focused on the condition of unidirectional solidification and planar S/L interface, most of which studied the interaction process between sole or several particles and solidification interface.\textsuperscript{6–9} Ode \textit{et al.}\textsuperscript{10} used phase field model to study particle/interface problem and critical velocity for pushing/engulfment transition for the system of Fe–C alloys and a silica particle. Under the common solidification condition, equiaxed dendritic structure is often occurred during the solidification of the SiC particle reinforced aluminum alloy. Particle shape, size, distribution and volume fraction all have important effects on final solidification structure and product performance. It is obvious that it has vital practical significance to simulate microstructure formation and evolution consider-
ing multi-particles pushing/engulfment phenomena. But it has seldom been reported so far on the composite microstructure simulation considering the particle pushing based on macro solidification.

The microstructure formation of SiC particle reinforced Al–7.0mass%Si composite made by stir casting was simulated in this paper. The present studies of this paper for solidification process of composite were divided into two parts: one was macro heat calculation which was carried out in the scope of real casting (in the order of magnitude of m), and the other was microstructure calculation which was carried out in the scale of μm. Because the computer can’t accomplish the full coupling in the scope of real casting according to the present capability, the author calculated macro heat based on the whole casting firstly, then selected one small area (one macro cell) to calculate microstructure. It means that two sets of meshes were used to carry out macro and micro calculation, respectively. It was a single-direction coupling between macro and micro calculation. Micro calculation was based on macro calculation, but the information of micro calculation such as micro solid fraction wasn’t fed back into macro parts. Two-dimensional models under normal solidification condition considering macro heat transfer, nucleation, equiaxed dendrite growth and particle pushing were presented in this paper. A modified cellular automaton method coupled with finite difference method was used to compute the grain growth. In addition, the effects of SiC particle volume fraction and different casting processes, pouring temperature and cooling rate on composite microstructure and particle distribution were analyzed. The simulated results were compared with those obtained experimentally.

2. Mathematical Formula of Al–Si/SiCp Microstructure Formation in Stir Casting

2.1. Physical Representation

Stir casting makes the reinforcements homogeneously distribute in melt through rotating movement of mixer, and then the molten metal is poured into the mould. Figure 1 is schematic diagram of stir casting process. As shown in Fig. 1, the stir casting process includes two stages: (1) melting and mixing. In this stage, matrix is melted in the crucible through heating equipment; reinforced particles are added into the matrix melt and mixed with melt together homogeneously through mechanical stirring. (2) Pouring. Composite melt got in the first step is poured into mould, and then solidifies into the final shaped casting. For simplicity, only the second stage is considered, which means starting to compute after the melt is poured into mould. An initial particle distribution is given randomly in advance. Figure 2 is the physical representation for microstructure simulation of particle reinforced composite. Two different grids are applied to compute macro heat transfer and microstructure respectively. Microscopic computation is based on macro heat transfer. Microscopic computing area has energy and solute exchange with its surrounding areas.

2.2. Main Assumptions of the Models

The main assumptions employed in the present models are as follows:

1. Two dimensional solidification with equiaxed microstructure;
2. Particle, liquid and solid are treated as separate phases;
3. The solid is rigid and stationary;
4. The particles are rigid and spherical and do not react chemically with the matrix. Further, the particles are assumed to be uniformly distributed in melt prior to solidification;
5. Local thermal equilibrium exists. The temperatures of liquid, solid and particles in one cell are equal;
6. Volume change during solidification is negligible;
7. All thermophysical properties are assumed to be constant.

2.3. Macro Heat Transfer Model

Two dimensional macro heat transfer model is based on heat conduction equation:

\[ \nabla \cdot \left( \kappa \nabla T \right) = \nabla \cdot \left( \Gamma _{\text{conv}} \right) + \Gamma _{\text{rad}} + \dot{Q} \]

Fig. 1. Schematic diagram of stir casting process: (a) melting and mixing; (b) Pouring. 1, SiC particle; 2, electric motor; 3, mixer; 4, crucible; 5, heating element; 6, melt; 7, mould; 8, composite.

Fig. 2. Physical representation for microstructure simulation of particle reinforced composite.
where \( \rho \) is the density, \( c \) is the specific heat, \( k \) is the thermal conductivity, \( T \) is temperature, \( t \) is time.

Composite includes the reinforced particles which make thermal and physical properties of the composites different with the matrix alloy. Thermal and physical properties and latent heat are modified according to the rule of mixture for composite properties.\(^{11,12}\)

(1) Conductivity:
\[
k_c = k_{ma}(1-V_p) + k_pV_p
\]
where \( k_c, k_{ma}, k_p \) are the thermal conductivity of the composite, matrix and particle, respectively; \( V_p \) is the particle volume fraction.

(2) Specific heat:
\[
c_c = c_{ma}(1-W_p) + c_pW_p
\]
where \( c_c, c_{ma}, c_p \) are the specific heat of the composite, matrix and particle, respectively; \( W_p \) is the particle mass fraction, \( W_p = \rho_pV_p/\rho_c \). The density of composite \( \rho_c = \rho_pV_p + \rho_m/V_m \); \( \rho_c, \rho_m, \rho_p \) are the density of the composite, matrix and particle, respectively.

(3) Latent heat:
\[
\text{Latent heat per unit mass for composite can be expressed as:}
\]
\[
L = L_m(1-V_p) + L_pV_p
\]
where \( L_m, L_p \) are the latent heat of the composite, matrix and particle, respectively.

The boundary condition at the casting/mould interface and the mould/air interface are given by

At the casting/mould interface:
\[
q = h_{cm}(T_{\text{casting}} - T_{\text{mould}})
\]
At the mould/air interface:
\[
q = h_{ma}(T_{\text{mould}} - T_{\text{air}})
\]
where \( q \) is the heat flux, \( T_{\text{casting}}, T_{\text{mould}} \) and \( T_{\text{air}} \) are the temperatures of the casting, the mould and the air at the mould surfaces, and \( h_{cm} \) and \( h_{ma} \) are the interfacial heat transfer coefficients at the casting/mould and the mould/air interface, respectively.

2.4. Dendrite Nucleation and Growth Model

Final microstructure of PRMMCs consists of both matrix grains and reinforced particles. Furthermore, casting performance depends on the interaction between growing crystal and embedded particles. Particle pushing/engulfment phenomena firstly depend on the solidification front advancement when dendrite is growing, so dendrite nucleation and growth model must be determined. The continuous nucleation model based on Gaussian distribution is used in the present study. In order to describe dendrite profile accurately, mathematical constructional method is used and a shape function is introduced:
\[
L(\theta) = L_m[A + (1 - A)\cos 4\theta]
\]
where \( A \) is shape factor; \( L(\theta) \) is the growing radius of a point at the curve shape; \( \theta \) is the angle between the growing direction of a point at the curve and \( x \) axis. \( L(t) \) is the integral of the growing velocity of dendrite tip along the whole growing time
\[
L(t) = \int_0^\pi v_t[\Delta T(t)]\,dt
\]
where \( v_t[\Delta T(t)] \), the growing velocity of dendrite tip, can be calculated by the KGT\(^{\text{TM}}\) model, which is also used in the following particle pushing model. The shape function can describe the grain profile well because it considers secondary dendrite. Besides, coordinate transformation method is used to treat the relationship between points and complex curve so that the equiaxed grain growth in the undercooled melt and the node capturing can be described better.\(^{14}\) Apparently, dendrite nucleation and growth model must consider the effect of particles. More details related to dendrite growth are explained in references.\(^{15,16}\)

2.5. Particle Pushing Model

As far as PRMMCs are concerned, when the moving S/L interface meets heterogeneous particles suspended in the melt, three different ways of the interaction between particles and approaching freezing front may appear: (1) particles are pushed away ahead of the moving front; (2) particles are engulfed in the front instantaneously; (3) particles are pushed for a while before being engulfed or entrapped by approaching dendrite arms.\(^{17}\) The particle–front interaction is very important for the final microstructure and the performance of composites. When particles are engulfed in the front, the final distribution of particles is the same as that of melt. If particles are pushed by the freezing front, they are dispersed or clumped in localized or ultimately solidified areas easily. This will lead to the decrease of ductility and fracture toughness. In general, pushing of the particle by the front is undesirable. So it is necessary to study the interaction between particles and the solidification interface and then establish particle pushing/engulfment model.

Influencing factors of particle pushing are as follows:
particle shape, size, volume fraction, thermal and physical properties of particle and matrix, interface shape, interface temperature and solute distribution and so on. Many criterions on particle pushing/engulfment have been presented to predict particle distribution, among which critical velocity criterion is applied extensively. The criterion thinks that there is a force balance between the particle and the solidification front. When a particle is approached by an advancing solidification front, the latter must obtain a certain "critical velocity" in order to engulf the particle. If the solidification velocity is below this critical value, the particle will be pushed, and if the front velocity is above this value, the particle will be engulfed. Even though this criterion is established under the condition of unidirectional solidification and planar solidification interface, it has vital theoretical meaning for particle distribution study under normal solidification condition.

Most of the ceramic reinforced particles can't act as nucleation substrate for PRMMCs. In addition, equiaxed dendrite solidification is the main solidification way for PRMMCs. Because solidification velocity is small for particles which can't act as the substrate, particles are always pushed. This is approved by the experimental results in the present study. So particle pushing phenomenon under normal solidification condition is studied in the paper, and the mathematical model coupled with macro heat transfer, dendrite nucleation and growth is established. Microstructure simulation of composite considering particle pushing is eventually realized.

As the solidification front approaches one particle, the particle is believed to experience both repulsive forces (which push the particle away from the front) and attractive forces (which push the particle towards the front). Under the action of the repulsive and attractive forces, if the particle can achieve a constant velocity equal to that of the solidification front, the whole system is said to reach a steady-state pushing mode until the particle meet with other matrix grains, other particles or the wall. Then the front and the particle move at the same speed with the particle being pushed ahead of the front, with a thin melt gap of constant thickness separating the two phases. The final gap thickness turns out to be a few hundred molecular diameters, which is about few tens of nanometers. So it is reasonable completely in the scale (micrometers) of the present study that the forces begin to interact between the solidification front and the particle once the matrix grains contact with the particles.

At the beginning of solidification, an initial particle distribution is given according to particle volume fraction and particle average diameter. Particle shape is represented by spherical shape. Figure 3(a) is the schematic of particle profile and mesh generation. Because particle diameter ranges from 15 to 25 μm and the size of micro cell is 2 μm, it needs to be classified into two sorts to treat mesh generation of spherical particle and cell marking: particle diameter is equal to the sum of even cells and odd cells, which corresponds with Figs. 3(b) and 3(c) respectively. As shown in Fig. 3, particle boundary cells, particle center cells, particle neighboring cells, grain growing direction and particle pushing direction are all marked with different signs. When the solidification front meets with reinforced particle, the particle and the solidification interface will begin to interact and then particle will be pushed. For the sake of simplicity, only four pushing directions (up, down, leftward, rightward) are considered here. As shown in Fig. 4, (a) the particle is immobile when $t=t_0$ and particle velocity $v_p=0$. (b) Left neighboring cells of the particle have been changed into matrix grain cell when $t=t_1$ initially ($t=t_1|_0$). (c) When $t=t_1$, ultimately, particle pushing direction is rightward and particle velocity is equal to $v(t_1)$, the growth velocity of dendrite tip at $t=t_1$. At this time, particle begins to be pushed. The displacement of the particle is based on the position change of particle center cell. So the new position of the particle can be determined when $t=t_2$ initially (as shown in (d), $t=t_2|_0$). At this time, particle velocity $v_p=0$ and upper neighboring cells of the particle have been changed into matrix grain cell. (e) When $t=t_2$ ultimately, particle pushing direction is down and particle velocity is equal to $v(t_2)$, the growth velocity of dendrite tip at $t=t_2$. At the next time step, the same judgment as that of the last time step is made until the particle meet with other matrix grains, other particles and the wall in the moving direction. All particles must

![Schematic diagram of particle profile and cell marking.](image)

**Fig. 3.** Schematic diagram of particle profile and cell marking. (a) Schematic of particle profile and mesh generation; (b) mesh generation and cell marking when particle diameter is equal to the sum of even cells; (c) mesh generation and cell marking when particle diameter is equal to the sum of odd cells.
be judged by the criterion of pushing at each time step. Particles’ positions are renewed with the growth of matrix grains until when solidification is over, the final composite microstructure is achieved.

In addition, the following problem must be solved during particle pushing. At one certain time step, if one particle meets with two or two more growing grains, it is firstly determined if different pushing direction caused by different growing grains’ action can meet the pushing criterion. Then one certain direction is randomly selected as the current pushing direction among all possible directions. If there are two opposite directions on one line, particle will be immobile along this line. The method accords with real physical mechanism according to the model itself and the simulated results. It means that the particle moves under the action of surrounding matrix grains. The present model decomposes the resultant forces acting on the particle, and only one component force is treated at each time step. Final particle moving track is in good agreement with real physical phenomenon.

3. Experimental Study

PRMMCs were produced by stir casting in this paper. Two casting processes were used here: sand and metal mould casting. Matrix material is Al–7.0mass%Si alloy and reinforced phase is industrial green α-SiC with average diameter of 20 μm. In order to study the effect of the cooling rate on microstructure, step-shaped sample castings were cast. 5 mm×5 mm specimen was cut from every step of the step-shaped sample casting. The height of the specimen was 50, 40, 30, 20, 10 mm respectively. 5% HF was selected as etching agent with 1–3 min etching time. The sample casting shape, size and the positions of the specimens are schematically shown in Fig. 5. Five specimens were indexed as 1#–5# in order according to the thickness of the step. Metallographs were obtained with an optical microscope after polishing and etching.

4. Simulated Results and Discussion

4.1. Composite Heat Transfer and Microstructure Simulation

Thermophysical data of Al–7.0mass%Si/SiC composite used in the calculation are presented in Table 1. Two-dimensional model under normal solidification condition considering macro heat transfer, nucleation, dendrite growth and particle pushing was presented in the above section. Solidification process of Al–7.0mass%Si/SiC composite produced by metal mould casting was simulated with 720°C pouring temperature and 5% particle volume fraction. The size of macro-cell for heat transfer is 1 mm×1 mm×1 mm, and is further divided into 500×500 CA cells for microstructure simulation. The measured and calculated cooling curves are shown in Fig. 6 (the modeling position is 3#). As shown in Fig. 6, the simulated results are in good agreement with the experimental results except a bit difference near the eutectic point. This is due to no special consideration for eutectic solidification. More explanations about eutectic simulation problem will be given in the Sec. 4.3.

The simulated results of the evolution of composite microstructure are shown in Fig. 7. At the beginning of solidification, an initial distribution of SiC particles is given. With the increase of undercooling, matrix grains nucleate and grow gradually. When the growing grains meet with the reinforced particles, they begins to interact, and whereupon particles are pushed. The growth of matrix grains is blocked due to reinforced particles. Finally, particles are
distributed at grains boundaries and the area solidified finally.

4.2. Comparison with Experimental Results

4.2.1. The Effects of Particle Volume Fraction and Casting Processes

Composite microstructures under the condition of sand mould and metal mould casting were simulated using the present model. The effects of SiC particle volume fraction and different casting processes on composite microstructure and particle distribution were analyzed. The simulated results are shown in Fig. 8.

As shown in Fig. 8, because of the faster cooling rate of the metal mould, the matrix grains are smaller. While the cooling rate of the sand mould is slower, the matrix grains are relatively bigger.

With the increase of SiC particle volume fraction, composite matrix grains are refined, but the action is not obvious. At low solidification rates such as the conditions of the described experiment of this paper, by decreasing the mass of the solidifying metal per unit volume and diminishing the quantity of liberated solidification heat, the particles introduced into the metal matrix can increase the cooling rates and decrease the solidification time. Besides, the growth of matrix grains is hindered by the reinforced particles. In general, the increase of particle content will refine the matrix grains.

Particle clustering phenomena all exist for different SiC particle volume fractions, but there are some changes on particle distribution homogeneity. There are more areas of particle clustering when the particle volume fraction is larger. But at the same time, the denuded areas without reinforced particles are fewer. Particles are uniformly distributed relatively in general. With the decrease of SiC particle volume fraction, the areas of particle clustering are diminished. But at the same time, the denuded areas without reinforced particles are increased greatly. So the extent of particle inhomogeneity is increased with the decrease of SiC particle volume fraction. As shown in Fig. 8, the simulated results are in good agreement with the experimental results.

4.2.2. The Effects of Pouring Temperature

The effects of pouring temperature on composite microstructure and particle distribution are presented in Fig. 9. As shown in Fig. 9, with the increase of pouring temperature, composite matrix grains are coarsened, which agrees with experimental results well. It can be easily explained that the solidification time is longer with the higher pouring temperature, which cause matrix grain to grow bigger.

When the pouring temperature is low, there are more areas of SiC particle clustering. With the increase of pouring temperature, the areas of particle clustering are diminished. Particles are distributed more uniformly. But the above action is not clear.
The effects of cooling rate on composite microstructure and particle distribution are presented in Fig. 10. For step-shaped sample casting in present study, the thickness of the step becomes thinner and the cooling rate becomes larger from 5# step to 1# step. As shown in Fig. 10, the higher cooling rate is, the more uniform particles are distributed. Besides, with the increase of the cooling rate, the matrix grain size is smaller. These trends can be understood due to the fact that the growth of secondary dendrite arm will interrupt particle movement and accumulation. The higher cooling rate is, the denser the secondary dendrite arms are, and the smaller the secondary dendrite arm space is. In general, the simulated results are in good agreement with those obtained by the experiment.

**4.3. About Eutectic Simulation**

Solidification structures of Al–7.0mass%Si alloy under equiaxed solidification condition include eutectic phase. At
the beginning of solidification, when the temperature is below the liquidus of alloy, equiaxed crystals nucleate in the melt. Primary $\alpha$-Al phase forms firstly and grows with dendrite shape. As the growth proceeds, secondary dendrites grow on the primary dendritic stems. Then solute accumulates between dendrites and interrupts the growth of dendrite here. Finally, Al–Si eutectic phase of high concentration forms between dendrites. Both simulated and experimental results in Ref. 20) showed that the primary $\alpha$-Al phase constituted the large percentage of solidification microstructure of Al–7.0mass%Si alloy and exhibited the dendritic structure when the pouring temperature was above 660°C. In the present study, the pouring temperatures of all kinds of conditions were above 660°C and the final major dendritic structure was validated by the experimental results. Eutectic phase appears at the final stage of solidification when the temperature decreases below eutectic point, which hasn’t obvious effect on the impingement between primary dendrites and particles as well as particle final distribution. On the other hand, the knowledge and quantitative understanding of eutectic solidification has remained very limited.21) It is very complex to simulate eutectic solidification of Al–7.0mass%Si alloy because it includes the nucleation of eutectic phase, cooperative and competitive growth of two eutectic phases (nonfaceted $\alpha$ phase and faceted $\beta$ phase), coupling between phase transformation and solute redistribution and so on.22) So the simulation of the primary dendrites growth and the interaction between grains and particles is vital to the present study and eutectic simulation is neglected in this paper. We will couple the present model with solute redistribution in the next work in order to simulate the solidification of Al–7.0mass%Si/SiC$_p$ composite more accurately.

5. Conclusion

The microstructure formation and particle distribution of SiC particle reinforced Al–7.0mass%Si composite made by stir casting was simulated in this paper. The following conclusions are obtained:

1) Two-dimensional models under normal solidification condition considering macro heat transfer, nucleation, dendrite growth and particle pushing were presented. The effects of SiC particle volume fraction and different casting processes on composite microstructure and particle distribution were analyzed. The simulated results were compared with the experimental results and they agreed with each other well.

2) The simulated results show that grain size is smaller for metal mould casting than sand mould casting. With the increase of SiC particle volume fraction, composite matrix grains are refined and particles are distributed more uniformly.

3) The simulated results show that composite matrix grain size becomes finer when the pouring temperature is lower. With the increase of pouring temperature, particles are distributed more uniformly.

4) The simulated results show that composite matrix grain size becomes finer when the cooling rate is larger. With the increase of cooling rate, particles are distributed more uniformly.

Acknowledgements

The research was sponsored by the National Significant Fundamental Research Project of the Ministry of Science and Technology of China (2005CB724105) and Nonferrous Metal New Material Key Laboratory Foundation from Lanzhou University of Science and Technology.

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