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Study of the channel segregation using a two-phase columnar solidification model

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Abstract. A two-phase columnar solidification model was used to study the formation mechanism of the channel segregation in a Sn-10 wt.% Pb benchmark ingot. The two phases considered in the current model are the melt and columnar phase. The morphology of the columnar dendrite trunks is approximated as step-wise cylinders with constant primary dendrite arm spacing. The growth kinetics of the columnar trunks is governed by the diffusion of the rejected solute element surrounding the columnar trunks. From the 3D modelling result one can ‘visualize’ the dynamic formation sequence of the channel segregation. The final channel segregation pattern shows a discontinuous and lamellar- or plume-structure. The formation mechanism of the channels is due to the disturbed flow, which can accelerate and retard the local solidification rate in the mushy zone and near the solidification front. This study has also verified that the channel segregation can form in the condition without remelting, namely, remelting is not a necessary condition for channel segregation.

1. Introduction
Channel segregation is one of the most frequently observed segregation pattern in different casting processes, such as large steel ingots, vacuum-arc remelting or electro-slag remelting ingots, etc. [1-2]. The generally termed channel segregation is often called as ‘A-segregate’ in large steel ingot [3], or ‘freckles’ in directionally solidified turbine blade [4]. In the early literature the ‘A-segregate’ was also termed as lamellar- or plume-shaped segregation [5-6].

People have experimentally studied the formation mechanism of the channel segregation for several decades [7-8]. Recently, numerical models [9-13] provided an alternative method to investigate the mechanism of channel segregation. A widely accepted explanation to the formation of the channel segregation is [5]: it is the perturbed fluid flow of the solute-rich interdendritic melt which causes the remelting of the dendritic fragments in the mush zone, hence to form the channel. Therefore, people generally believe that the channel originate from and develop with remelting.

Modeling of channel segregation is a multiphase and multiscale problem. The most promising model is the multiphase volume-averaging approach pioneered by Beckermann and co-workers [14-15]. The two-phase columnar solidification model used here is a simplified version of the mixed columnar-equiaxed solidification model, which was developed by two of the current authors [16-18], by ignoring the appearance of the equiaxed phase. Details of the numerical model for the columnar solidification are described elsewhere [19].

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2. Model description

Figure 1 shows a 2D configuration of the benchmark ingot (Sn-10 wt.% Pb), together with necessary boundary and initial conditions. Both 3D and 2D calculations are made. For the 3D simulation all the boundary conditions are the same as the 2D case except for the front and back walls for which we applied the non-slip condition for the fluid flow calculation, and a convective cooling condition for the heat transfer coefficient, $h$, equal to 50 W m$^{-2}$ K$^{-1}$ with an external temperature ($T_{\text{EXT}}$) of 298 K. All the thermophysical properties, boundary conditions and numerical parameters used in this study are given in literature [20].

Details of the numerical model for columnar solidification are described elsewhere [17, 19]. A brief outline of the model assumptions is given below.

- Two phases are included in the model: the melt and the columnar dendrite trunks.
- The morphology of the columnar dendrite trunks is approximated by step-wise cylinders, and the primary dendrite arm spacing, $\lambda_1$, is constant. The arrangement of the cylindrical columnar trunks is assumed to be staggered.
- The columnar trunks initially grow from the casting surface when constitutional undercooling is achieved. Solidification front coincides with the liquidus isotherm.
- The liquid-to-solid mass transfer (solidification/melting) rate, $M_\ell$, is calculated based on the radial growth velocity of the columnar trunks, $v_R$, which is governed by diffusion of solute element in the interdendritic melt surrounding each cylindrical trunk.
- A linearly binary Sn-Pb phase diagram with a constant solute redistribution coefficient, $k$, and a constant liquidus slope, $m$, is used.

3. Simulation results and discussions

3.1. 3D solidification results

Examples of the transient 3D simulation result at 100 seconds are shown in figure 2(a)-(b). In figure 2(a), the velocity vectors were shown in two planes (a vertical central plane and a horizontal plane with a distance of 0.01 m from the bottom), together with liquid volume fraction isolines. Figure 2(b) predicted the $c_{\text{mix}}$ in gray scale (dark for the highest and light for the lowest value) with $c_{\text{mix}}$-isolines in the vertical central plane and the streamlines (arrows for flow direction) of the melt flow are also overlaid in this plane. For the alloy considered in the simulations (Sn-10 wt.% Pb), the interdendritic melt enriched with Pb solute element has a higher density than the bulk melt, and both the thermal and solute buoyancy forces lead to a downward flow along the solidification front. The resultant solute-enriched melt tends to create a downward flow near the solidification front, subsequently to form a clockwise circulation in the whole cavity, as seen in figure 2(b). The liquid flow is obviously seen in the region where the liquid fraction is bigger than 0.4, while in the region where the liquid fraction is smaller than 0.3 the liquid velocity is unapparent. It means that the liquid melt can hardly flow through the dendritic mushy region where the liquid fraction is smaller than 0.3. When channels are initiated in
the mush zone, the velocity fields (see paths of the streamlines) will be significantly changed. As the liquid volume fraction inside the channel is higher than in the neighbouring regions, the permeability of the channels is relatively higher. Therefore, the interdendritic melt would take preferentially its path along the channel, and the streamlines are periodically diverted.

![Image of velocity and liquid fraction](image1)

**(a) velocity & liquid fraction**

![Image of c_mix and streamlines](image2)

**(b) c\text{\textsubscript{mix}} & streamlines**

**Figure 2.** 3D results at 100 s. (a) velocity vectors shown in two planes (a vertical central plane and a horizontal plane with 0.01 m from bottom), together with liquid volume fraction isolines in the vertical central plane; (b) predicted \(c_{\text{mix}}\) in gray scale and \(c_{\text{mix}}\)-isolines in the vertical central plane, the streamlines (arrows for flow direction) of the melt flow are also overlaid in this plane.

Transient development of the flow channels during solidification can be ‘visualized’ in figure 3. The iso-surfaces of liquid volume fraction \(f_\ell = 0.35\) are plotted. The regions enveloped in these iso-surfaces, where \(f_\ell\) is bigger than 0.35, indicate the channels. The channels are 3D in nature, discontinuous, and lamellar-structured. They occur only in the right bottom region, which takes only a quarter of the whole calculation domain. The channels originate from the region adjacent to the cooling wall, and develop with a certain angle (about 40 - 60 degrees to the horizontal plane). The channel space (distance between neighbouring channels) is almost constant, or slightly adjusted with the time during solidification.

The global solidification sequence shows that in the upper part of the ingot the solidification front, approximated with the iso-surface of \(f_\ell = 0.35\), sweeps much faster than in the bottom region. The explanation for this is that the downward flow in the mushy zone transports the Pb-rich interdendritic melt from the upper to the bottom region; hence the liquidus temperature in the upper region is increased and in the bottom region is depressed. As a consequence the solidification rate in the upper region is accelerated, and in the bottom region is retarded.
Figure 3. Predicted 3D solidification sequence from (a) 30 s to (d) 400 s. The liquid volume fraction in two planes (a vertical central plane and a horizontal plane with a distance of 0.01 m from the bottom) is shown in colour scale. The iso-surfaces of liquid volume fraction \( f_i = 0.35 \) are shown to demonstrate the formation sequence of the flow channels.

The final macrosegregation profile of this ingot is predicted and shown in figure 4. Globally, negative segregation is predicted in the upper-right region, and positive segregation is predicted in the low-left region. The minimum and maximum values of \( c_{\text{mix}} \) in this calculation are 0.03 and 0.35 of Pb in mass fraction, respectively. Channel segregation pattern is clearly seen. The structure of the channel segregates (inclined angle, channel space, number of the channels) corresponds to the previous analysis of figure 3.

Figure 4. Distribution of mixture mass fraction of Pb at the end of the solidification.

3.2. The formation mechanism of the channel segregation

If we further assume that in the current columnar solidification model the diffusion within a local volume in the interdendritic melt region is infinitive, then we have [21],

\[
\frac{\partial c_i}{\partial t} = -(1-k) \frac{c_i}{f_i} \frac{\partial f_i}{\partial t} - u_i \cdot \nabla c_i. \tag{1}
\]
From $T = T_i + M \cdot \sigma^s$, we get
$$\frac{\partial c^*_i}{\partial t} = \frac{1}{m} \frac{\partial T}{\partial t}$$  \hspace{1cm} (2)

Equation (3) minus equation (2),
$$\frac{\partial (c^*_i - c_i)}{\partial t} = \left(1 - k\right) \frac{c_f}{f} \frac{\partial f}{\partial t} + \frac{1}{m} \frac{\partial T}{\partial t} + u \cdot \nabla c_i.$$  \hspace{1cm} (3)

In the LHS of equation (3), $(c^*_i - c_i)$ is the driving force for solidification/melting, which governs the solidification/melting rate, $M_m$ [17]. Therefore, the local solidification/melting is actually induced by three contributions, corresponding to the three RHS terms of equation (3). The 1st RHS term is the contribution of the solidification-induced solute enrichment of the interdendritic melt, the sign of which is always negative with the progress of solidification. The solidification rate decreases with the enrichment of solute in the interdendritic melt. The 2nd RHS term is the contribution of cooling rate, the sign of which is always positive. It means that the solidification rate increases with enhanced cooling. The 3rd term is what we called perturbation term, $u \cdot \nabla c_i$. Its sign can be positive or negative, depending on the interdendritic flow, as schematically shown in figure 5. In the mush zone, where the melt flows in the direction of the concentration gradient, the above term is positive. It means that the local solidification rate is accelerated; hence this zone is called a solidification-accelerated zone. On the contrary, in the mush zone, where the melt flows in the opposite direction of the concentration gradient, the above term is negative. It means that the local solidification rate is retarded; hence this zone is called a solidification-retarded zone. The physical explanation to the contribution of the perturbation term is as follows. The interdendritic melt flow modifies the local concentration of the melt, $c_i$, which in turn changes the driving force for the solidification $(c^*_i - c_i)$.

Channel segregations occur in the solidification-retarded zone. In this zone, the increase rate of the volume fraction solid, $f^*_s$, is lowered down by the retarded solidification, hence to induce a relative low $f^*_s$ in comparison to the neighbouring zones where the perturbation term is positive. The relative lower $f^*_s$ in this zone will enhance the flow, as the permeability increases with the decrease of $f^*_s$. Further on, the perturbation term would become more negative due to the enhanced flow (equation (3)), and the local solidification rate becomes even smaller. As a consequence, the ratio of the local $f^*_s$ to the $f^*_s$ of its neighbouring zones becomes smaller and smaller, hence a channel is initiated. This mechanism is verified by the current modeling results, as detailed in figure 6. In this figure the red colour indicates the positive value of $u \cdot \nabla c_i$, and the blue shows the negative value of $u \cdot \nabla c_i$. The blue zones, where the values of the perturbation term $u \cdot \nabla c_i$ are negative (in another word, the direction of interdendritic velocity vector, $u$, and the liquid concentration gradient vector, $\nabla c_i$, is opposite), are the solidification-retarded zones. As discussed above, the solidification rate in these solidification-retarded zones is decreased by the flow, hence is the value of solidification (mass transfer) rate, $M_m$, in these solidification-retarded zones very small, namely, 20 - 40 kg·s⁻¹·m⁻³. In comparison the solidification rate, $M_m$, is very high (as high as 160 kg·s⁻¹·m⁻³) in the solidification-accelerated (red) zones. As a consequence, channels are initiated from the solidification-retarded (blue) zones. One interesting finding is that the channels occur without
evidence of remelting, i.e. \( M_{\ell c} \geq 0 \). Additionally, it is noted that the streamlines change their direction abruptly when they reached the channels. The streamlines are diverted in the direction of the channels.

![Image of analysis of the formation mechanism of the channel segregation.](image)

**Figure 6.** Analysis of the formation mechanism of the channel segregation. Only the relevant simulation results zoomed in the right bottom of the mould cavity are shown (\( t = 40 \) s). (a) Contour of \( \vec{u} \cdot \nabla c_\ell \) in red (positive) and blue (negative), overlaid by the isolines of mass transfer rate, \( M_{\ell c} \). (b) Contour of liquid fraction, overlaid by the vectors of liquid velocity and the streamlines (black). (c) Contour of \( c_{\text{mix}} \) in mass fraction.

Moore and Shah [5] have also discussed the above-mentioned mechanism of channel segregation. Recently, Sawada et al [22] have studied the mechanism of the channel segregation in the vertical directional solidification with a Pb-10 wt.% Sn alloy, and got a similar conclusion about the solidification accelerated and retarded regions.

4. Conclusion

The 3D simulations with a two-phase columnar solidification model have ‘visualized’ the transient development of the channel segregation in the benchmark ingot (Sn-10 wt.% Pb). Channel segregation appears near the wall-bottom corner. The final channel segregation pattern shows a discontinuous, and lamellar- or plume-structure.

It is verified by the current model that the remelting is not the necessary condition for the formation of channel segregation. Although remelting is not predicted in the current benchmark, the channel segregation still appears. The origin of the channels is due to the flow perturbation. The numerical study has shown the strong co-relation of the local solidification rate to the perturbation term, \( \vec{u} \cdot \nabla c_\ell \). If the perturbation term becomes locally negative, the solidification rate will be significantly retarded there, hence to promote the initiation of a channel. In return the newly initiated channel will strengthen the flow perturbation, the perturbation term becomes more negative, and the channel becomes more stable.

Acknowledgments

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