The fine scale convection in the boundary layer mode is called "fingers." Fingers in aqueous NH₄Cl appear before channels form, but when the channels and their plumes develop the fingers disappear. Hence, if the same sequence occurs in Pb-Sn alloys, then our channels would appear to simulate reality. Of course, channels are three-dimensional, but Neilson and Incropera[4] indicate that channels can be simulated by both two and three dimensional calculations. Finally, if our so-called pockets are channels, then their lifetimes are too short. Channels in both metallic alloys and aqueous NH₄Cl solutions persist over much longer distances. Felicelli et al.[10] showed that channels within the mushy zone persist when flow lateral to the wall of the channel is inhibited. This suggests that a mechanism involving a large reduction of permeability at the wall of the channel might be responsible for stabilizing the internal channels.

ACKNOWLEDGEMENTS

The authors are grateful to NASA-MSAD for the support of this work. Computations were done at the San Diego Supercomputer Center with a grant provided by CRAY Research Inc. The code was developed by Dr. S. Felicelli, now with Centro Atomico Bariloche in Argentina. Mr. N. Kulkarni, graduate student, and Dr. J. Crempien of the University of Concepcion, Chile, ably assisted the authors.

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For the autonomous directional solidification process, shell molds which are made of SiO₂-free ceramics covered inside with a nucleation inhibiting amorphous layer are used. After casting the melt into the shell mold, the heater device is switched off. The temperature of the melt decreases, and, due to the amorphous front layer, the nucleation is delayed, leading to a substantial undercooling. The isolated water-cooled chill plate at the bottom of the shell mold ensures a longitudinal temperature gradient within the melt and the nucleation to occur at the coldest position within the foot of the specimen. The isolation between the metal and the chill plate is realized with a ceramic plug. According to the thickness of this plug the temperature gradient can vary between nearly zero and more than 1 K/mm. Both limiting cases can lead to a single crystal solidification (2). Figure 1 shows the geometry of a cylindrical sample solidified as a single crystal by ADS with the corresponding cooling curves measured at various positions. The cooling rate within the melt is about \( T = 0.25 \) K/s and the temperature gradient is \( G = 0.82 \) K/mm. The solidification starts at the bottom of the specimen with an undercooling of about \( \Delta T_{\text{mu}} = 30 \) K.

The single crystal produced by ADS consists of several large columnar dendrites (2). Within the present model, it is assumed that the dendritic growth is parallel to the specimen axis and that the same growth conditions can be applied for each dendrite. The longitudinal and the lateral growth is considered separately. Because of the geometry of the problem cylindrical coordinates are used.

According to W. Kurz and D.J. Fisher 1989 (10) the following relation between the growth rate \( v \) and the undercooling at the dendrite tip \( \Delta T^* \) has been used:

\[
v = \frac{D}{\pi^2 \mu \Delta T_0} \Delta T^* \quad (1)
\]

where \( D \) is the diffusion and \( \Gamma \) the Gibbs-Thomson coefficient, \( \mu \) is the distribution coefficient and \( \Delta T_0 \) the solidification interval.

The corresponding tip radius \( R \) is given by (10)

\[
R = 2 \pi \left( \frac{\Delta T}{\Delta T_0} \right)^{1/2}
\]

The longitudinal growth of the dendrite tip is followed by the lateral growth of the dendrite arms. In the present model, the radial growth is treated as a 2D-equiaxed growth, and thus a modified 2-dimensional Rappaz-Thévoz model has been worked out. Because most of the rejected solute is pushed radially, it is assumed that the mass transport in longitudinal direction can be neglected. Thus the solute distributions within a transversal section may be said to be independent of the neighboring sections.

Considering a cylindrical volume element with a radius \( R_l \) and a thickness of unity, as shown in Fig. 2, the radial fraction of the dendritic evolution \( f_g \) and the solid fraction \( f_s \) may be related to the corresponding radii \( R_l \) and \( R_s \) by:

\[
f_g = \left( \frac{R_g}{R_l} \right)^2 \quad \text{and} \quad f_s = \left( \frac{R_s}{R_l} \right)^2.
\]

Based on similar assumptions as made by M. Rappaz and P. Thévoz (complete mixing of solute within the interdendritic liquid, uniform temperature of the grain, etc.) the solutal balance within the cylindrical volume element results in the same expressions for the internal fraction \( f_i \) and for the solute layer thickness \( s \).

Figure 1: Specimen geometry of a single crystal produced by ADS and cooling curves measured at different positions.

Figure 2: Schematic of the longitudinal and the transverse section of a dendrite with the corresponding solute distribution.
The following differences to the Rappaz and Thévoz model have been seen to exist.

Based on the expression for solutal conservation:

\[
(c^* - c_0) \pi (R_g^2 - R_d^2) = \int_{R_d}^{R_g} \frac{c^* - c_0}{\delta} (R_g + \delta - R_d) 2\pi R dR
\]  

(4)

\(f_g^r\) is related to \(f_g\) by:

\[
f_g^r = f_g \cdot g(x) = f_g \left(1 + \frac{1}{3}x^2\right),
\]

(5)

with

\[Z = \frac{\delta}{R_g}.
\]

(6)

\(f_g^r\) is defined in Fig. 2 (\(R_g\) is the corresponding radius). This relationship between \(f_g\) and \(f_g^r\) is slightly different to that obtained in the spherical growth model (5).

Another difference appears in the energy equation. In the present paper the conduction of heat between the various cylindrical volume elements has been included. Thus the energy equation is given by:

\[
2\pi R_d Q + \pi R_d^2 \lambda \frac{\Delta T}{\Delta x^2} = \pi R_d^2 \left(\rho c_p \frac{\Delta T}{\Delta t} + L \frac{\Delta \xi}{\Delta t}\right)
\]

(7)

in which \(Q\) is the external heat flow in lateral direction, \(\lambda\) the thermal conductivity, \(\rho c_p\) the volumetric specific heat, \(L\) the volumetric latent heat and \(\Delta T\) the change in temperature within the time step \(\Delta t\). For relating the change in the supersaturation \(\Delta \Omega\) to \(\Delta T\) the following expression is used:

\[
\Delta T = m_0 c^* \equiv \Delta \Omega (k_0 T_0)
\]

(8)

Based on the above equations the evolution of \(T, f_g^r\) and \(f_g\) can be calculated as a function of the solidification time until the radial solute layer reaches the total lateral radius \(R_t\). To describe dendritic impingement the solute concentration at \(R_t\) has to increase as soon as the boundary layer approaches \(R_t\). An appropriate description has been implemented into the model.

The advance of the dendrite in longitudinal direction is calculated by using the simple relation:

\[
x^d = x^o + v \cdot \Delta t
\]

(9)

where \(x^o\) and \(x^d\) is the old and the new tip position, respectively. The velocity has been calculated using equation (1) by considering that the tip undercooling \(\Delta T^s\) is estimated by a linear interpolation between the temperatures of the neighboring transversal sections.

It is assumed that the solidification starts at the bottom of the specimen (first volume element) at an undercooling of \(\Delta T_{Nu} = 15\,\text{K}\) with a nucleus, \(R_{Nu} = 5 \cdot 10^{-6}\,\text{m}\) in size. The nucleation conditions for the further cylindrical volume elements are assumed to be:

i) \(\Delta T_{Nu}\) due to the temperature of the considered volume element which is reached by the longitudinal growth.

ii) \(R_{Nu}\) due to the radius of the corresponding dendrite tip.

As in the other models the presented algorithm originates from describing the microstructure evolution of binary alloys. To apply the algorithm in the case of superalloys the multi-component system has been reduced to a quasi-binary alloy (11). On this score the diffusion coefficient \(D\) is estimated by applying the constitutional undercooling criterion (12):

\[
D = \frac{\Delta T_{Nu}}{(G/v)^2}\]

(10)

where \((G/v)^2\) is the critical \(G\) over \(v\) value for the appearance of constitutional undercooling. \(G\) is the temperature gradient at the liquid/mushy interface. The distribution coefficient \(k\) is approximated as:

\[
k = \frac{v_c}{v_l}
\]

(11)

in which \(v_c\) and \(v_l\) are the critical velocities for the morphological transition planar-cellular and cellular-dendritic (13).

The values of \((G/v)^2, v_c\) and \(v_l\) for the superalloy CMSX-6 have been previously estimated by D. Ma 1990 (14). The resulting \(D\) and \(k\) together with other relevant physical properties of the superalloy CMSX-6 are listed in Table 1.

Table 1: Physical properties used in the calculation for the superalloy CMSX-6

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquidus temperature (T_L)</td>
<td>1336°C</td>
</tr>
<tr>
<td>Diffusion coefficient (D)</td>
<td>(2.9 \times 10^{-9}) m²/s</td>
</tr>
<tr>
<td>Distribution coefficient (k)</td>
<td>0.31</td>
</tr>
<tr>
<td>Solidification interval (\Delta T_{Nu})</td>
<td>100 K</td>
</tr>
<tr>
<td>Heat of fusion (L)</td>
<td>(1.5 \times 10^8) J/m³</td>
</tr>
<tr>
<td>Gibbs-Thomson coefficient (\Gamma)</td>
<td>(10^{-7}) Km</td>
</tr>
<tr>
<td>Heat capacity (\rho c_p)</td>
<td>(9.17 \times 10^8) J/(m³ K)</td>
</tr>
<tr>
<td>Heat conductivity (\lambda)</td>
<td>30 W/Km</td>
</tr>
</tbody>
</table>
RESULTS AND DISCUSSION

Figure 3 shows the calculated cooling curves and the solid fraction vs. time curves at various positions within a cylindrical specimen similar to that in Fig. 1. A cooling rate of $T = 0.25$ K/s and a temperature gradient of about $G = 1.2$ K/mm have been applied. The undercooling at the onset of solidification has been assumed to be $\Delta T_{NV} = 15$ K. Due to this undercooling the cooling curve, calculated at the bottom of the specimen, has a remarkable recalculation. At higher positions the solidification starts with smaller undercooling, and thus the recalculation is less pronounced. This result is in good agreement with the experimental measurements (Fig. 1).

![Figure 3: Calculated cooling and solid fraction curves corresponding to the thermocouple locations 1, 2 and 3 in Fig. 1.](image)

Figure 4 shows the calculated temperature distribution and the corresponding solid fraction curves within the cylindrical sample for two different initial temperature gradients. With a large gradient of $G = 1.2$ K/mm the initial undercooling of about $\Delta T_{NV} = 15$ K is restricted to a small area at the bottom of the specimen (Fig. 4a). A recalculation can only be determined within this region (compare curve 1 in Fig. 3). Unless this transient solidification rate is governed only by the heat flow - the growth condition emerge to directional solidification. As the release of latent heat reduces the temperature gradient in the mushy region, the expression $v = T/G$ gives only an upper limit for the solidification rate. In Fig. 4a the growth rate $v$ is about 0.19 mm/s whereas $T/G$ is 0.21 mm/s. The solid fraction increases monotonously due to the advance of the liquid/mushy interface (Fig. 4b).

Applying a small gradient of about $G = 0.01$ K/mm (Fig. 4b) a quasi homogeneous undercooling within the entire specimen can be achieved before the onset of solidification. This results in uniform growth conditions along the specimen (constant growth rate, equal recalculation and uniform solid fraction evolution). The solidification rate is determined by the growth into the undercooled melt. According to equation (1) $v$ is about 0.8 mm/s. After the longitudinal growth the entire specimen has become a homogeneous mushy zone in which the temperature as well as solid fraction are uniform.

![Figure 4: Calculated distribution of temperature and solid fraction along the specimen at different times for two different initial temperature gradients of $G = 1.2$ K/mm (a) and $G = 0.01$ K/mm (b). The numbered arrows in (a) correspond to the cooling curves in Fig. 3.](image)
Conclusion

Based on the solid diffusion model by M. Rappaz and P. Thévoz 1987 an approach has been made to study the lateral growth of the dendrite arms in the mushy zone during autonomous directional solidification. A modified cylindrical model was proposed in which the longitudinal growth of the dendrite axis and the heat accumulation in longitudinal direction was considered. The calculated cooling curves at various locations show different depth of recrystallisation which is also observed in the measurements.

Acknowledgement

The authors would like to acknowledge to Dr. J. Stanescu for numerous discussions concerning ADS experiments and for measuring the cooling curves in Fig. 1.

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