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Modelling of soft impingement during solidification

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Abstract. **It has been well established that spheroidal grain morphology in the microstructure forms during stir casting (rheocasting) and grain refinement of magnesium alloys by zirconium addition. This curious microstructure has been of interest both commercially from enhanced mechanical properties and also scientific interest in explaining the mechanism of spheroidal grain formation. Vogel and Doherty proposed a model describing the fracturing of dendrite arms during stir casting to produce a high density of nuclei which they presume to give rise to spheroidal grains. They proposed that there is soft impingement of diffusion fields of neighbouring nuclei, which reduces the concentration gradient ahead of the planar solid and liquid interface, which in turn negates shape instability. In this paper, the Vogel and Doherty model is pursued by quantitative modeling of soft impingement problem and related to shape instability by constitutional supercooling theory. This analysis correctly predicts the spheroidal grain formation during stir casting or rheocasting. This model can also be used to explain the grain refinement of magnesium alloys by zirconium addition wherein spheroidal grains are formed.**

Keywords. **Spheroidal grains; stir casting; diffusion fields; impingement.**

1. Introduction

It is well established that cast microstructure after stir casting or rheocasting is novel in that it has spheroidal grains with the absence of dendrites which is normal microstructure in castings.

Spheroidal grain morphology of cast structure is very predominant during stir casting (rheocasting) and also grain refinement of Mg alloys by zirconium addition. For example, Kattamis *et al* (1967) showed in magnesium alloys where grain size was reduced to that of the dendrite arm spacing, that spherical grain structure and segregation pattern were produced. Similarly, fragmentation of dendritic growth by stir casting produces a spherical morphology of solidification microstructure (see for example, Spencer *et al* 1972; Joly and Mehrabian 1976).

In generalizing a suggestion by Vogel (1976) made in the context of the stir casting process, it has been pointed out by Doherty (1982) that when there is a high density of nuclei growing with full diffusion control, then a stable non-dendritic growth form may be expected when the overlapping diffusion fields from adjacent growing crystals interact to reduce the concentration gradient that causes shape instability (Doherty *et al* 1984). Figure 1 shows the effect of stir casting on the microstructure of an Al alloy.

It has also been shown by Flemings (1974) that a spheroidal grain morphology occurs during grain refinement of Mg alloys by Zr addition. Since the micro-segregation pattern is different with a spheroidal grain structure than a dendritic structure, an enhancement of mechanical properties is expected. With this background, the objective of this paper is to explain on the basis of constitutional supercooling theory, the soft impingement of diffusion fields due to a high density of nucleation either during stir casting or grain refinement.

2. Mathematical model

Kurtz and Fisher (1998) proposed a solution for the diffusion field of a moving interface in 2D under steady state conditions.

The standard Fick's second law is modified, to take into consideration the advance of the interface, under the following transformation

$$z = x - vt, \tag{1}$$

where z is the moving reference frame, x the spatial coordinate, v the velocity of the interface and t the time as explained by Kurtz and Fisher (1998).

This transformation when applied to Fick's second law gives the directional growth equation

$$\frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} + \frac{v}{D}\frac{\partial C}{\partial z} = 0. \tag{2}$$

A solution to the above equation is arrived at by considering the following boundary conditions:

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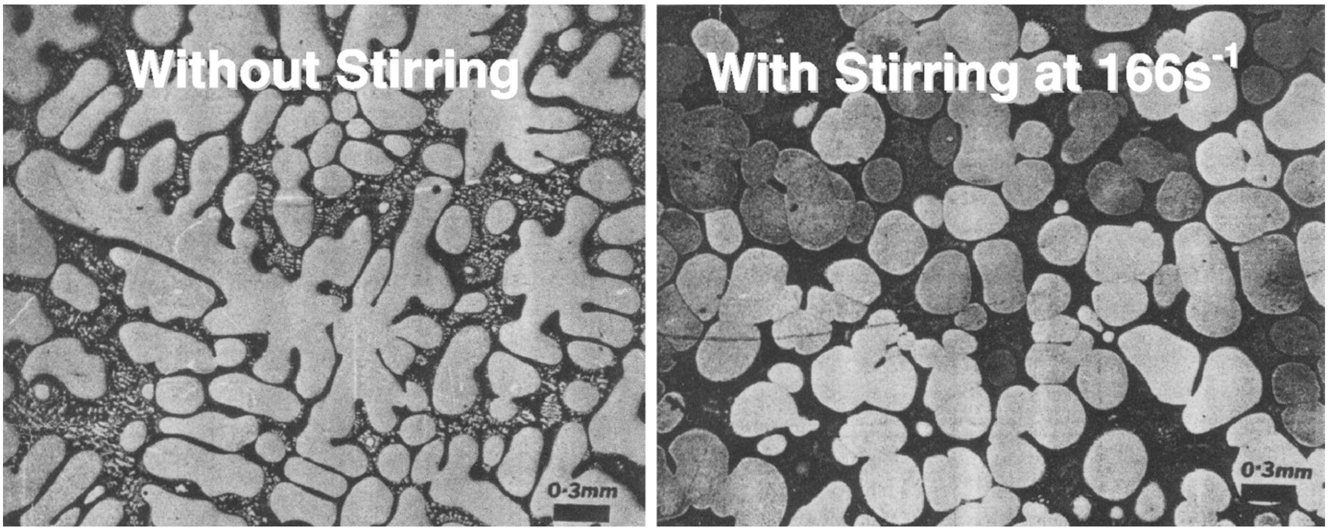

Figure 1. Al–1·5wt.%Cu cooled at 40°C $\min^{-1}$ from above the liquidus to 588°C and held isothermally for 3 h before quenching (Doherty 1982).

(i) The region far ahead of the interface is unaffected by the interface advance; hence, the Dirichlet condition can be applied

$$C = C_0 \text{ at } z \to \infty. \tag{3}$$

(ii) Due to symmetry of the interface along the y axis, the Neumann condition can be applied

$$\frac{\partial C}{\partial y} = 0. \tag{4}$$

The Robin condition is not required for solution and the method of Laplace transforms is used in developing the solution to the partial differential equation which is a one-dimensional equation and by virtue of the Neumann condition, there is no lateral diffusion.

The resulting solution is as follows:

$$C_{\mathrm{I}} = C_0 + \left(\frac{C_0}{k} - C_0\right) e^{-\frac{v}{D}z}. \tag{5}$$

Till now only a single interface has been considered; hence, another second interface is considered at a distance of Δ from the first interface. This second interface is moving in the opposite direction with a velocity, $-v$. The velocity and nature of the two interfaces are considered to be identical. Thus, the directional growth equation for the second interface is given by applying the same transformation

$$\frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} - \frac{v}{D}\frac{\partial C}{\partial z} = 0\,. \tag{6}$$

On assuming similar boundary conditions, the solution for the second interface is obtained by the method of Laplace transforms as follows

$$C_{\mathrm{II}} = C_0 + \left(\frac{C_0}{k} - C_0\right) e^{-\frac{v}{D}(\Delta - z)}. \tag{7}$$

The resultant diffusion field of both interfaces can be arrived at by the principal of superposition

$$C_{\mathrm{sum}} = C_{\mathrm{I}} + C_{\mathrm{II}}$$

$$= 2C_0 + C_0\left(\frac{1}{k} - 1\right)\left[e^{-\frac{v}{D}z} + e^{-\frac{v}{D}(\Delta - z)}\right]. \tag{8}$$

The above equation gives a solution for the diffusion field of two interfaces converging on each other. This is similar to the growth of two adjacent nuclei, in stir casting. In this case, Δ would represent the inter nuclei spacing.

The constitutional supercooling theory states that if the interface morphology is 'bumpy', i.e. irregular, and if the liquid thermal gradient is less than $m(\mathrm{d}C_{\mathrm{sum}}/\mathrm{d}z)$, then the tip of these bumps will experience greater supercooling than the rest of the body. Such a situation facilitates the bumps to grow and leads to dendritic growth. Conversely, if the thermal gradient in the liquid is equal or more than $m(\mathrm{d}C_{\mathrm{sum}}/\mathrm{d}z)$, then there is no thermal advantage to promote dendritic growth; hence, such a condition facilitates a planar solid–liquid interface, resulting in non-dendritic growth (figure 2).

Thus, the following equations provide the limiting condition for a spheroidal grain structure to result on solidification of an alloy.

$$\frac{\mathrm{d}T}{\mathrm{d}z} = m\frac{\mathrm{d}C_{\mathrm{sum}}}{\mathrm{d}z}, \tag{9}$$

$$\frac{\mathrm{d}C_{\mathrm{sum}}}{\mathrm{d}z} = \frac{v}{D}\left(\frac{C_0}{k} - C_0\right)\left[e^{-\frac{v}{D}(\Delta - z)} - e^{-\frac{v}{D}z}\right]. \tag{10}$$

From the above condition, it is possible to determine the liquid thermal gradient for a series of Δ. Δ can be related to the concentration of nuclei by considering a random array of nuclei in the melt. In such a case it becomes more appropriate to consider Δ as the Gaussian mean of nuclei size.

The above calculations were performed for Al–7Si and Al–4Cu systems, and the data used is as shown in table 1.

3. Results

The diffusion fields of the two interfaces are shown overlapping each other in figure 3 and the resultant diffusion field is shown in figure 4 for Al–4Cu system with $\Delta = 0{\cdot}01$ cm. The calculated thermal gradients are tabulated in table 2. From the table it can be seen that for Δ values < 10 μm in Al–4Cu and 1 μm in Al–7Si, $m(\mathrm{d}C_{\mathrm{sum}}/\mathrm{d}z)$ is lower than the imposed liquid temperature gradient of ~30–50°C/cm. Hence, as per the constitutional supercooling theory, non-dendritic growth occurs producing spheroidal grain structures.

Another conclusion that comes from these results is that Al–4Cu alloy shows a greater frequency of spheroidal grains than Al–7Si alloy which has to be verified experimentally.

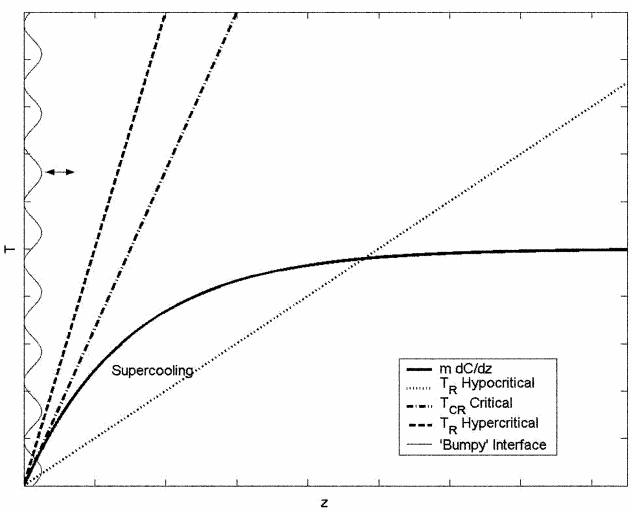

Figure 2. Condition for shape instability and stability as per constitutional supercooling.

Table 1. Data used for calculations.

	Al–7Si	Al–4Cu
D	1×10^{-5} cm²/s	1×10^{-5} cm²/s
C_0	0·07	0·04
m	−6·6	−3·406
k	0·11	0·173
v	$2{\cdot}5 \times 10^{-3}$ cm²/s	$2{\cdot}5 \times 10^{-3}$ cm²/s

The above results point to the need of a critical density of nuclei below which Δ is small so no dendritic growth occurs. This critical density is achieved in stir casting and grain refinement of magnesium alloys by zirconium addition. Doherty (1982) showed that in stir casting the secondary dendrite arms are severed from the main trunk of the dendrites due to recovery and recrystallization and formation of high angle grain boundaries in the dendrite arms. The liquid aluminium then wets the high angle grain boundaries thus severing the secondary arms from the main trunk of dendrites. These severed arms constitute the high density of nuclei for further heterogeneous nucleation. This constitutes to the high density on nuclei in stir casting. If the nuclei are sufficiently close to each other, then the above mathematical model of the two-interface problem is valid where the diffusion fields overlap each other and homogenize concentration thus negating the constitutional supercooling. This is the reason why

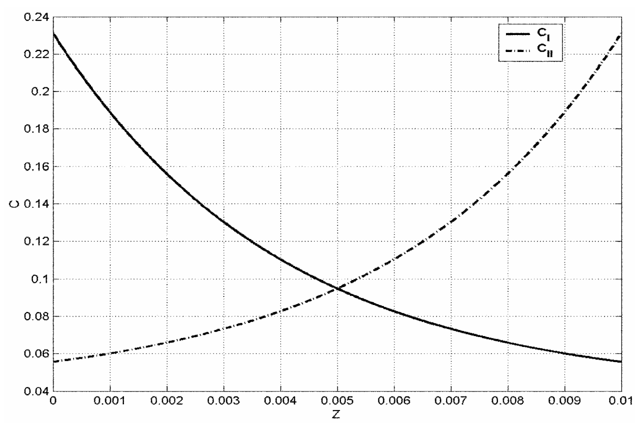

Figure 3. Diffusion fields of converging interfaces, Al–4Cu system, $\Delta = 0{\cdot}01$ cm.

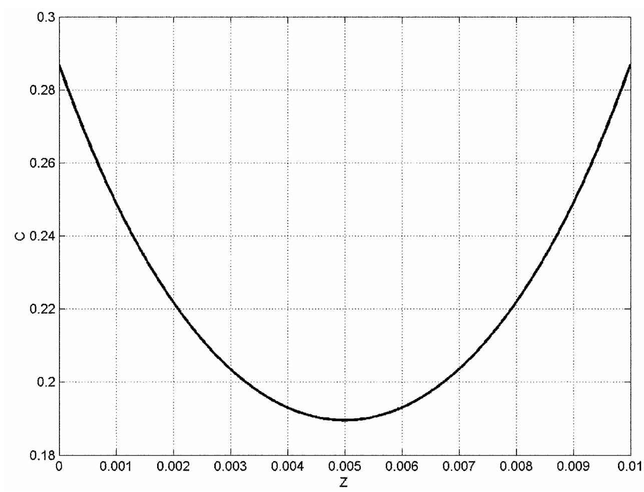

Figure 4. Resultant diffusion field, Al–4Cu system, $\Delta = 0{\cdot}01$ cm.

Table 2. Calculated thermal gradients.

	Al–4Cu	Al–7Si
Δ (μm)	$m(\partial C/\partial z)$ (°C/cm)	$m(\partial C/\partial z)$ (°C/cm)
0·1	0·340	2·333
1	3·364	23·073
10	30·136	206·711
100	125·057	857·792
1000	136·240	934·500

lack of dendrite morphology is observed in stir casting and only spheroidal grains are observed.

4. Conclusions

From the above analysis, it is clear that the presence of a high density of nuclei is responsible for the shape stability of the interface which results from soft impingement of diffusion fields of neighbouring nuclei. Hence, this is the necessary condition which must be achieved in stir casting (rheocasting) and grain refinement of magnesium alloys by zirconium addition. This model constitutes a rigorous validation of Vogel and Doherty's model of soft impingement of diffusion fields during rheocasting and a similar problem of grain refinement of magnesium alloys by zirconium addition. The mathematical model in the present paper gives an analysis of the formation of the spheroidal grains during rheocasting by soft impingement of diffusion fields from neighbouring nuclei during nucleation and growth during solidification.

Nomenclature:

z, Direction along interface advance;
y, direction perpendicular to interface advance;
v, velocity of interface;
D, diffusion coefficient;
C_0, solid composition;
k, equilibrium distribution coefficient;
m, liquidus slope;
C, concentration in wt %.

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