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A simple model for dendrite arm coarsening during solidification in multicomponent alloys

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The mechanical properties of a casting are largely dependent on secondary dendrite arms spacing, since it determines the solute segregation, the final distribution of inter-dendrite phases, and porosity [1]. Owing to the remelting and resolidification mechanism, dendrite arm coarsening contributes significantly to homogenization during solidification. While a large number of analytical and numerical studies of the dendritic solidification of binary alloys exist [2], few attempts have been made toward developing a model for multicomponent alloys.

Roósz, Kraft *et al.* [3, 4] have presented numerical models for the prediction of dendrite arm coarsening in multicomponent alloys. The back diffusion in the solid must be determined by using a time consuming finite difference scheme. In this paper, the back diffusion behavior is easily solved by introducing the diffusion layer thickness. After comparing the results of this simple solution with the experimental results of former researchers, it is shown that this simple model is satisfactory for the prediction of dendrite arm coarsening during the solidification process.

Coarsening of the secondary dendrite arms is described by the semi-empirical relationship in binary alloys [3]:

$$[\lambda(t)]^3 - \lambda_0^3 = \int_0^t BM(T)\,\mathrm{d}t \qquad (1)$$

where $\lambda(t)$ is the secondary dendrite arm spacing and λ_0 is its initial spacing. B is a geometric factor relating curvature differences to λ and $M(T)$ includes all temperature dependent terms. Taking the dendrite coarsening results of Kattamis [2], Roósz has defined the coarsening parameter $M(T)$ as

$$M(T) = \frac{\gamma D_\mathrm{L}}{\Delta Hm(1-k)C_\mathrm{L}} \qquad (2)$$

where γ is the energy of solid/liquid interface, ΔH is the latent heat of solidification, m is the liquidus slope, k is the solute partition coefficient, D_L is the solute diffusion coefficient in liquid phase and C_L is the solute composition in liquid phase.

Roósz, Kraft *et al.* have extended this model to multicomponent alloys by assuming that the coarsening process at each time step is governed by the element with the lowest value of $M_\mathrm{i}(T)$, the subscript i refers to element i, i.e.,

$$M(T) = \min\{M_1(T), M_2(T), \ldots, M_\mathrm{n}(T)\}. \qquad (3)$$

Generally this is the element with the lowest liquid diffusion coefficient.

The evolution of the solute profiles in the volume element is shown schematically in Fig. 1.

During the time interval of dt, the solid/liquid interface moves by ds and the length of the volume element X increases by dX because of an increase in dendrite arm spacing. Coarsening is thus considered by using a volume element increasing in length according to

$$X(t) = \lambda(t)/2 \qquad (4)$$

where $\lambda(t)$ is given by Equation 1.

For each solute, the mass balance yields

$$C_{\mathrm{L,i}}(1-k_\mathrm{i})\,\mathrm{d}s = (X-s)\mathrm{d}C_{\mathrm{L,i}} + (C_{\mathrm{L,i}} - C_{0,\mathrm{i}})\mathrm{d}X + D_\mathrm{s}\frac{\partial C_\mathrm{s}(s,t)}{\partial x}\mathrm{d}t. \qquad (5)$$

The back diffusinon flux during the time interval in solid phase, i.e., the shaded square A_4 in Fig. 2 can be approximately described as [5]

$$A_4 = D_\mathrm{s}\frac{\partial C_\mathrm{s}(s,t)}{\partial x}\mathrm{d}t = \frac{1}{2}\delta_\mathrm{s}\mathrm{d}C_\mathrm{s}^* \qquad (6)$$

where δ_s is the diffusion layer thickness and can be described as

$$\delta_\mathrm{s} = \frac{2D_\mathrm{s}}{V} \qquad (7)$$

where V is the interface velocity, i.e., $V = \mathrm{d}s/\mathrm{d}t$. In the analysis, the local equilibrium condition at the solid/liquid interface has been applied, i.e., $C_\mathrm{s}^* = kC_\mathrm{l}$, where k is the solute partition coefficient.

So the solute balance for each solute i can be written as

$$C_{\mathrm{l,i}}(1-k_\mathrm{i})\,\mathrm{d}s = (X-s)\,\mathrm{d}C_{\mathrm{l,i}} + (C_{\mathrm{l,i}} - C_{0,\mathrm{i}})\mathrm{d}X + \frac{k_\mathrm{i}D_\mathrm{s}}{V}\mathrm{d}C_{\mathrm{l,i}}. \qquad (8)$$

The relationship between cooling time t, temperature T, and amount of solid phase m_s, is given by the heat

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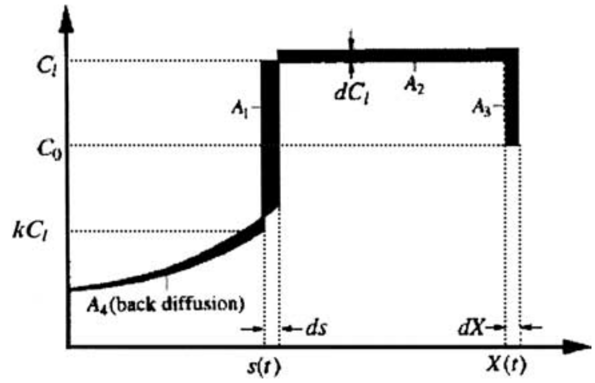

Figure 1 Solute concentration in a solidifying volume element with coarsening.

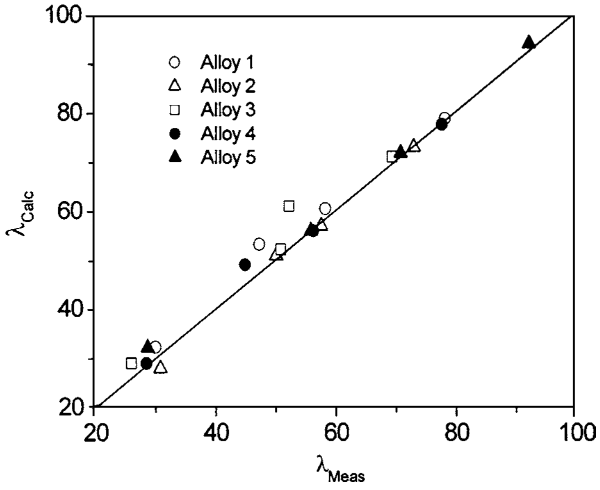

Figure 2 Comparison of calculated dendrite arm spacings and experimental values.

balance. Taking into the account the heat content of the crucible, we get

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = \Delta H \frac{\mathrm{d}m_\mathrm{s}}{\mathrm{d}t} + (m_\mathrm{s} S_\mathrm{s} + m_\mathrm{l} S_\mathrm{l} + m_\mathrm{c} S_\mathrm{c}) \frac{\mathrm{d}T}{\mathrm{d}t}. \quad (9)$$

The heat flux during solidification can be calculated from the cooling rate at liquidus temperature, $\dot{T}_\mathrm{l}$, according to

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = \frac{\dot{T}_\mathrm{l}\ (m_\mathrm{l} s_\mathrm{l} + m_\mathrm{c} S_\mathrm{c})(T - T_0)}{T_\mathrm{l} - T_0}. \quad (10)$$

If $T(t)$ is known from the cooling condition, the solute compositions are readily determined by the phase equilibrium relation, i.e.,

$$T = T_\mathrm{m} + \sum_{i=1}^{n} + m_\mathrm{i} C_\mathrm{l,i} \quad (11)$$

During a time interval Δt, the temperature may change to $T(t + \Delta t)$ according to the cooling curve. The increase of the secondary dendrite arm spacing can be determined by Equation 1. By assuming a little movement of the solid/liquid interface, ds, the solute compositions can be deduced form the mass balance Equation 8. So the system temperature can be obtained from the phase equilibrium relation, i.e., Equation 11. Its difference from the calculated temperature by Equations 9 and 10 should be less than 0.1 K. If this is alright, the numerical process could be carried out during the next time interval. If it is not, ds should be adjusted until the temperature criterion is satisfied.

The initial conditions for Equation 8 are specified as follows:

$$s(t = 0) = X(t = 0) = 0; \quad C_\mathrm{L,i}(t = 0) = C_\mathrm{0,i}. \quad (10)$$

Here, the application of this model to the industrial Al—Cu—Mg alloys is executed in detail. The experimaental results of five Al—Cu—Mg alloys obtained by former researchers [6] are used to demonstrate the applicability and precision of this model. The compositions and cooling rate at liquidus temperature are given in Table I. The values of physical constants used in the calculation are listed in Table II.

TABLE I Compositions and cooling rates at the liquidus temperature of different alloys

	Composition (wt%)		Cooling rate (Ks^{-1})			
Alloy no.	Mg	Cu	1	2	3	4
1	1.35	3.98	18.1	3.97	2.70	1.08
2	0.94	4.11	21.3	2.69	2.70	1.27
3	0.45	4.00	18.5	3.91	2.63	1.60
4	0.87	5.07	18.7	3.71	2.61	0.90
5	0.98	3.12	22.1	1.08	2.34	1.08

TABLE II The physical parameters used in the calculation

Parameters	Unit	Value
$D_\mathrm{l,cu}$	m^2·s^{-1}	1.05×10^{-7} exp(−2860/T)
$D_\mathrm{l,Mg}$	m^2·s^{-1}	9.90×10^{-5} exp(−8600/T)
$D_\mathrm{s,Cu}$	m^2·s^{-1}	0.29×10^{-4} exp(−15600/T)
$D_\mathrm{s,Cu}$	m^2·s^{-1}	0.37×10^{-4} exp(−14900/T)
S_s	J·Kg^{-1}·K^{-1}	1.14×10^3
S_l	J·Kg^{-1}·K^{-1}	1.14×10^3
S_C	J·Kg^{-1}·K^{-1}	1.17×10^3
ΔH	J·Kg^{-1}	3.97×10^3
γ	J·m^{-2}	0.093

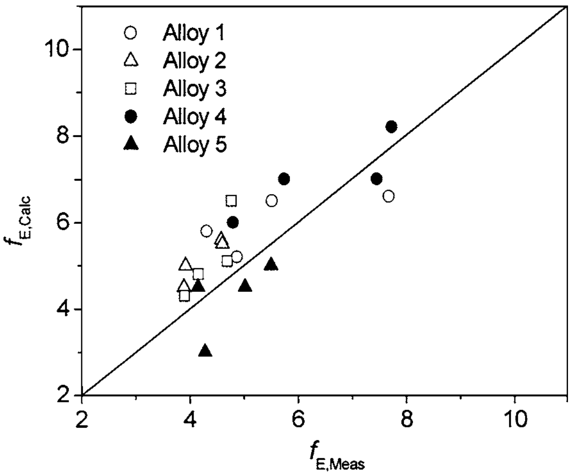

Figure 3 Calculated vs. measured amount of eutectic.

In Fig. 2, the experimental and the calculated secondary dendrite arm spacings are shown. Very good agreement between the measured results and calculated values has been achieved.

The calculated and experimental amounts of eutectic values are shown qualitatively in Fig. 3. The calculated eutectic amounts agree reasonably well with the measured values.

By introducing the diffusion layer thickness, the back diffusion behavior is easily solved without the time consuming finite difference scheme. The application of the simplified model to Al—Cu—Mg alloys is studied in detail. The good agreement between the experimental results and the calculated values shows that this simplified model is satisfactory for the prediction of dendrite arm coarsening during solidification in multicomponent alloys.

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