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Lateral heat flux and remelting during growth into the mushy-zone

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ABSTRACT

In the context of dendritic rapid solidification, the goal of this work was to develop a model that describes growth of the stable phase in the presence of a preexisting metastable phase without requiring in-depth knowledge of the local geometry of the growing dendrite or the growth environment. Results facilitate predictive computational materials modeling of the transformation sequence, solidification path and microstructural evolution during industrial casting operations. The model was evaluated using mushy-zone growth velocity data from Fe–Co and Fe–Cr–Ni alloys. The Fe–Co alloys that were tested are hyper-peritectic compositions, while the Fe–Cr–Ni alloys were evaluated as pseudobinary hypoeutectic compositions. The results show that for a given heat flux there will be a minimum undercooling for which dendritic growth can be supported. The predicted growth velocity which corresponds to that minimum undercooling agrees reasonably well with the measured experimental growth velocity data suggesting that the growth of the stable phase into the mushy zone occurs under the minimum conditions required to support dendritic growth.

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1. Introduction

Advanced materials are a cornerstone in nearly every field of technology. From consumer electronics to unmanned space vehicles, breakthroughs in materials science play a pivotal role in facilitating innovation. In 2011 the Materials Genome Initiative was implemented in the United States, with the main goal of reducing the amount of time that it takes to discover, develop, manufacture, and deploy new materials [1]. One critical mechanism for creating advanced materials is the ability to utilize simulation-based engineering effectively during the development process. Computational models have a proven track record of reducing the time and cost of development. The Committee on Integrated Computational Materials, of the National Academy of Sciences, provided a thorough investigation of the use computational materials engineering with multiple case studies [2]. While modeling aluminum castings, Ford Motor Co. benefited from a 15–25% reduction in development time and a significant reduction in cost. General Electric, Pratt & Whitney, and Boeing saw a 50% reduction in development time, and the amount of testing was reduced by up to a factor of eight.

There are two key components that are required for successful

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computational materials modeling: Accurate material properties, and a model that successfully describes the phenomena of interest. Containerless processing methods, such as electrostatic levitation (ESL), or electromagnetic levitation (EML), provide a means of accurately measuring various material properties, and observing solidification phenomena under conditions that would otherwise be unachievable. In this case, the phenomenon of interest is known as double recalescence. Containerless processing allows a molten sample to undercool below the liquidus temperature of the stable γ -phase (FCC) over a wide composition range for Iron-Cobalt and Iron-Chromium-Nickel alloys. If the undercooling is sufficient, i.e. the temperature is below the melting point of the metastable δ -phase (BCC), the sample can solidify in a two-step process known as double recalescence. In the event of double recalescence, dendrites of the metastable BCC δ -phase grow into the undercooled liquid, and the stable FCC γ -phase grows subsequently into the combination of primarily formed metastable solid and remaining undercooled liquid, or mushy-zone [3–10].

Matson and Hyers [11] previously addressed the growth of the stable phase into the mushy zone within an adiabatic remelt (AR) model. The model considers that there is some heat flux into the preexisting metastable phase, and that the heat extraction by remelting the metastable solid enhances dendrite growth rates. However, the model is dependent on knowing the thickness of secondary stable phase. The next step was to develop a model that sufficiently described growth of the stable phase into the mushy



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zone, without requiring in-depth local knowledge of the geometry of the growing dendrite or the growth environment.

In this article, we discuss a new method of evaluating solidification interactions when a secondary solid phase grows into a preexisting solid phase in a non-symbiotic manner, i.e., when the secondary phase remelts the primary phase. The mushy-zone growth velocity was assessed using a modified version of Lipton-Kurz-Trivedi (LKT) theory [12], including the kinetic undercooling component from Boettinger-Coriell-Trivedi (BCT) theory [13]. The model considers remelting of the pre-existing metastable δ -phase, as well as conduction from the tip of the stable γ -phase dendrite.

2. Experimental methods

The model was evaluated using Fe–Co and Fe–Cr–Ni data from the historical archive of previous containerless processing experiments. The Fe–Co data, including details regarding the experimental setup, can be found in Refs. [14,15]. The Fe–Cr–Ni data, and a description of the experimental setup, can be found in articles by Matson et al. [9,10].

3. Analysis

The measured mushy-zone velocity was assessed using a modified Lipton-Kurz-Trivedi (LKT) theory [12], incorporating the marginal stability criterion from Trivedi and Kurz [16], and including non-equilibrium effects related to solute trapping from Aziz and Kaplan [17], and kinetic effects from BCT theory [13].

When dendrites of the stable phase grow through the undercooled metastable mushy zone, they grow at a faster rate than they would through liquid at the same undercooling. This could be explained, in part, by an effective change in the heat capacity of the growth environment as described by the Adiabatic Remelt Model [11]. Fig. 1 shows a graphical representation of a stable phase dendrite growing into the mushy zone. Region 1 represents the preexisting liquid, and region 2 is the pre-existing solid, which is partially melted.

3.1. Accounting for remelting

In the following energy balance, exothermic reactions will be taken as negative and endothermic reactions will be taken as positive. If there is no heat flux back down the length of the and the growing dendrite.

$$Q_1 = \left(-\Delta H_{f,S} + C_P^L \Delta T_{SM}\right) \boldsymbol{V}_1 \tag{1}$$

 $\Delta H_{f,S}$ is the heat of fusion of the stable phase, C_P^L is the liquid heat capacity, ΔT_{SM}^{-1} is the difference in the liquidus temperatures of the stable and metastable phases, and V_1 is the corresponding volume in region 1 where the reaction occurs. Fig. 3 shows that the stable phase dendrite grows alongside the existing metastable phase. If the metastable phase acts as a chill, then the heat released from the dendrite tip in the primary growth direction will be reduced by the quantity J_S/V . A graphical representation of a dendrite growing through the mushy zone, with lateral heat flux from the tip, is given in Fig. 2.

 J_S is the heat flux conducted laterally such that it does not need to be rejected from the tip in the growth direction; *V* is the resulting growth velocity. The lateral heat flux is mathematically comparable to what Koseki [7] used while evaluating dendrite growth during chill casting. The net energy into region 1 for this case is given in Equation (2).

$$Q_1 = \left(-\left(\Delta H_{f,S} - J_S/V\right) + C_P^L \Delta T_{SM}\right) \boldsymbol{V}_1$$
(2)

Region 2 will absorb the remaining heat. The preexisting solid will melt and then the liquid will be heated. The net energy into region 2 is shown in Equation (3).

$$Q_2 = \left(\Delta H_{f,M} + C_P^L \Delta T_{SM}\right) \boldsymbol{V}_2 \tag{3}$$

 $\Delta H_{f,M}$ is the heat of fusion of the metastable phase, and V_2 is the corresponding volume in region 2 where the reaction occurs.

Absent other long-range heat transfer, conservation of energy requires that the sum of Equations (2) and (3) is equal to zero, as shown in Equation (4).

$$Q_1 + Q_2 = \left(-\left(\Delta H_{f,S} - J_S / V\right) + C_P^L \Delta T_{SM} \right) \boldsymbol{V}_1 + \left(\Delta H_{f,M} + C_P^L \Delta T_{SM} \right) \boldsymbol{V}_2 = 0$$
(4)

Solving for the ratio of V_2 to V_1 results in Equations (5) and (6)



Fig. 1. Graphical representation of a stable phase dendrite growing into the mushy zone.

dendrite, then in region 1 the growing dendrite will release energy equivalent to the heat of fusion, and the pre-existing liquid will absorb as much energy as can be allowed by the liquid's heat capacity and the temperature difference between the existing liquid

¹ For the alloys that were tested, the γ-phase is the stable phase, and the δ-phase is the metastable phase. Therefore, the subscript *SM* corresponds to γδ.

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