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A front-tracking model to predict solidification macrostructures and columnar to equiaxed transitions in alloy castings

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Abstract

The solidified grain structure (macrostructure) of castings is predicted by process simulation using a newly extended front-tracking technique which models the growth of solid dendritic fronts through undercooled liquid during metallic alloy solidification. Such fronts are either constrained, as is the case with directed columnar growth from mould walls, or unconstrained, as is the case for multiple equiaxed growth from individual nucleating particles distributed throughout the liquid. Non-linear latent heat evolution is treated by incorporating the Scheil equation. Thermal conductivity changes with the solid fraction. A log-normal distribution of activation undercooling to initiate free growth from equiaxed nuclei is used, and the routines to deal with such growth followed by impingement of dendritic grains upon one another are verified by comparison with the results of analytical studies of simplified systems. The extensions to the model enable the predictions of equiaxed grain structure and, importantly, the columnar to equiaxed transition in inoculated alloy castings. The model is validated via comparison with experimental results. The front-tracking method is proposed as a suitable formulation for modelling alloy castings that solidify with a dendritic structure, either columnar, equiaxed, or both.

Keywords: Solidification; Nucleation; Dendritic growth; Front-tracking

1. Introduction

Cast alloys may contain elongated columnar crystals, equiaxed crystals or, often, both. The metallic crystals form the grains of the cast component and the arrangement of these grains is known as the macrostructure. Metallurgists are interested in knowing the as-cast macrostructure because its nature influences the final properties of the material. In particular, metallurgists may want to know if there is a columnar to equiaxed transition (CET). CET charts are in existence for one-dimensional Bridgman furnaces [1,2]. These charts give the thermal gradients and solidification velocities required for the formation of an equiaxed zone. In industrial castings the foundry engineer can only influence the thermal gradients and solidification velocities indirectly. Hence, precise control of the macrostructure and CET in castings is more difficult than

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in the Bridgman setup. Direct simulation of the solidifying shape casting is required to determine the final macrostructure. Solidification models, which calculate the as-cast structure at different length scales, have been developed to predict the CET. Models that predict the columnar and equiaxed zones macroscopically (i.e., at the scale of the casting) include those by Wu and Ludwig [3], Martorano and Biscuola [4], and Jacot et al. [5]. Mesoscale models that predict the as-cast CET structure at the scale of the grain include a Monte Carlo model [6] and the cellular automaton finite element method [7]. Models that predict CET by calculating at the microscale (i.e., at the scale of the dendritic features) include the cellular automaton finite difference method [8] and the phase field method [9]. A good review of CET modelling techniques was recently given by Spittle [10].

A complete direct simulation of the industrial casting process will require a modelling domain that is at the scale of the casting process ($\sim$ m). Also the domain will have to be resolved down to the length scale of the solid–liquid interface, or approximately a length scale of the order of the dendrite tip radius ($\sim$ μm). Voller and Porte-Agel [11] investigated the resolution and size of grids from models presented in the literature. Comparisons were made to a Moore's law analysis. Their findings showed that, according to Moore's law, complete and direct simulation of industrial size castings across the wide range of length scales (μm to m) shall not be available until decades from now because of limitations of computer power.

Browne and Hunt [12] presented details of a front-tracking model (FTM) for modelling dendritic alloy solidification at the scale of the grain envelope (mm). Hence, modelling at the scale of the casting with FTM is convenient when compared to models that require grid resolution down to the scale of the solid–liquid interface. Two independent, but similar, FTM algorithms were described: one for dendritic columnar growth and one for dendritic equiaxed growth. Columnar solidification usually originates at the casting mould wall, where the free energy barrier to nucleation is lowered. The columnar structure consists of an array of elongated grains with a preferred orientation into the casting cavity. In FTM a moving computational front represents the growing dendritic columnar array. No crystallographic details on the individual dendrites are required; thus reducing the computational overhead with negligible effect on the predicted columnar front position [13].

On the other hand, equiaxed dendritic crystals are individual crystals that are assumed to nucleate in the melt at a location where the free energy barrier to nucleation is reduced, for example, at a foreign particle in the melt. In FTM each equiaxed dendrite is surrounded in a mesoscopic computational envelope that is defined to wrap around the dendrite tips (Fig. 1). As with the columnar front, no crystallographic or microscopic detail is required by the model; thus, again, reducing computational overhead.

Fig. 2 shows two schematic diagrams. Fig. 2a represents dendritic solidification of both dendritic columnar and dendritic equiaxed growth. A mushy zone is defined as a region that contains both liquid and solid. Two distinct mushy zones are identified, namely, the columnar mushy zone and the equiaxed mushy zone. The columnar mushy zone exists between the columnar dendrite tips and the completely solid region. The solid region may be defined by the eutectic temperature isotherm. The equiaxed mushy zone consists of the group of unconstrained equiaxed dendrites in the bulk melt.

Fig. 2b shows how the system of Fig. 2a is represented in FTM. It is clearly demonstrated that the columnar region is modelled at the macroscale of the casting, whereas the individual equiaxed crystals are modelled at the mesoscale of the grain envelope; thus, there is a bridging of the length scales.

Both columnar and equiaxed solidification fronts are modelled in the domain of the casting. The domain is divided into a fixed orthogonal grid. The solidification fronts are defined by computational markers at the intercepts of the fronts with the grid. The columnar front and equiaxed envelopes are mathematically described by piecewise linear segments between these markers. During growth of the crystals, a displacement vector, z_t, is calculated for each marker. The vector's direction is governed by the geometry of the front and its magnitude is given by Euler integration of the dendrite tip growth rate, v_t. In FTM, the dendrite growth rate must be written in terms of tip undercooling, ΔT, where

$$v_t = f(\Delta T). \tag{1}$$

Rebow and Browne [14] demonstrated the use of various growth rate laws with a columnar FTM. For our purposes we shall use the growth law of Burden and Hunt [15] approximated for low thermal gradients, which gives