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Simulation of the columnar-to-equiaxed transition in directionally solidified Al–Cu alloys

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Abstract

A combined cellular automaton-finite difference model was applied to simulate the columnar-to-equiaxed transition (CET) during the directional solidification of Al–Cu alloys. This model provided a novel insight into the solutal interactions both within the advancing columnar dendritic network and within the equiaxed grains forming ahead of them. Simulations revealed that solute interaction among secondary and tertiary arms is strong, but the interaction at the columnar tips is weak. The region with the largest solute adjusted undercooling was found to be in the region between columnar dendrites, rather than ahead of their tips as assumed in prior CET models. In addition, it was found that prior simulations which neglect the solute built-up at the interface predict the CET at a significantly lower velocity for a given gradient. The effect of crystallographic orientation on CET was also simulated and was found not to be significant. The influences of thermal gradient and growth rate on CET were combined on a CET map, showing good agreement with prior theoretical models at low growth rates, while at high growth rates the current model predicts that CET will occur at lower gradients. Reasonable agreement with the limited number of experimental observations available was obtained.

Keywords: Columnar-to-equiaxed transition; Solidification microstructures; Modeling; Directional solidification; Aluminum alloys

1. Introduction

Dendritic structures are prevalent in cast alloys, contributing significantly to the final properties of components manufactured from them. The dendrites can be part of either a columnar or equiaxed grain structure depending upon the local thermal and solutal fields. Columnar dendrites often grow from near the mould surface where the thermal gradients are high, transforming to an equiaxed structure when the gradient is reduced near the centre of the casting. Determining if the structure will be columnar or equiaxed is important. For example, in the direct-chill casting of aluminum alloys, equiaxed grains are desirable. Therefore, innoculation of the melt with heterogeneous nuclei is widely used to promote the columnar-to-equiaxed transition (CET). Conversely, in directionally solidified or single crystal superalloy turbine blade castings, columnar dendritic structures are desired; equiaxed grains are treated as casting defects because the high angle grain boundaries formed reduce creep rupture life. In these castings a columnar-dendritic structure is achieved using high thermal gradients and low growth rates, inhibiting the CET. In summary, understanding CET is important for the control of grain structures in solidification processes.

The columnar-to-equiaxed transition has been investigated for many years and numerous mechanisms have been proposed. In 1984, Hunt [1] developed the first analytical model to predict CET, based on the potential for equiaxed grains to nucleate in the constitutionally undercooled region ahead of the columnar front. He assumed that if the volume fraction of equiaxed grains

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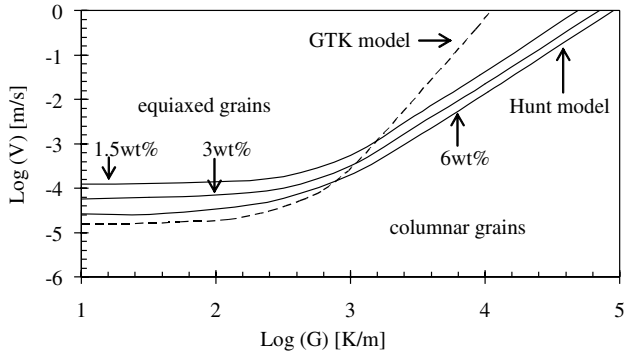

Fig. 1. Analytic model predicted CET. Solid curves: Hunt model for Al–1.5 wt% Cu, Al–3 wt% Cu and Al–6 wt% Cu alloys [1]. Dashed curve: GTK model for Al–3 wt% Cu [4]. ($\Delta T = 0.75$ K and $N_{max} = 1.0 \times 10^9 m^3$.)

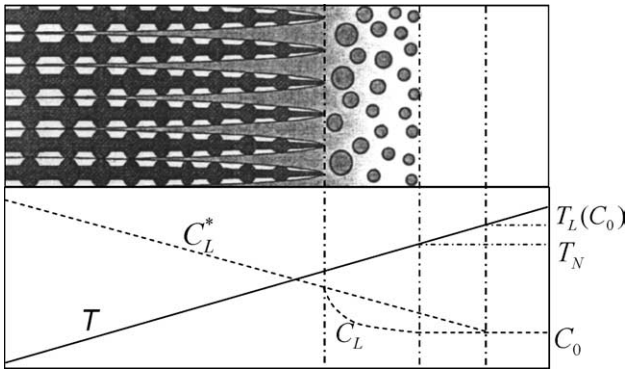

Fig. 2. Schematic of the solutal interaction between the columnar dendrites and equiaxed grains in the modified single domain CET model (after [2]).

exceeds 0.49, then the columnar dendrites will be blocked. Hunt calculated the solid fraction within the columnar zone using the truncated Scheil Equation [2,3] together with an empirical relationship to relate tip undercooling to alloy composition and cooling rate. Hunt's model was modified by Gäumann, Trivedi and Kurz (GTK model) in 1997 [4] by updating the analytical dendritic growth model to include non-equilibrium effects, extending its application to rapid solidification. The predicted columnar-to-equiaxed transition for Cu alloys using both Hunt's model and the GTK model are shown in Fig. 1. Both models predict the same relationship between CET and the key processing parameters of composition, thermal gradient and pulling velocity. The transition occurs more easily when an alloy has a high solute concentration, low thermal gradient and high pulling velocity. The predicted CET is similar for both models at conventional casting conditions but differs at high growth velocities.

In 1996 Wang and Beckermann [5] proposed a single-domain model to predict CET. In this single-domain model, three phases (i.e., solid, interdendritic liquid and extradendritic liquid) are separated by an imaginary solid/liquid (S/L) interface within a representative elementary volume (REV). Within an REV, the fraction solid change was predicted by solving both heat and solute conservation equations, predicting a slightly different evolution of the solid in comparison to the Scheil Equation [6]. However, equiaxed grains were assumed to form at the liquidus temperature without nucleation undercooling, and initial alloy concentration was employed to calculate the equilibrium temperature at the columnar front; consequently solutal interactions ahead of the advancing columnar dendrites were neglected. In 2003, Martorano et al. [7] coupled a solutal blocking mechanism into the single domain model. A schematic illustration of the mechanism simulated is shown in Fig. 2. Directional solidification was characterized by an applied temperature gradient across the domain and equiaxed grains were assumed to form at a fixed undercooling. The rejection of solute as the equiaxed grains grow was accounted for by increasing the solute concentration (C_L) ahead of the dendrite tips above the bulk liquid concentration (C_0). This resulted in a reduction of undercooling ahead of the columnar front. If the reduction was sufficient, the growth of columnar-dendrites would be blocked (termed as "solutal blocking"), and CET would occur. However, the gradient in solute between adjacent columnar dendrites was not considered.

In 1994, Gandin and Rappaz [8] proposed a stochastic model to simulate the grain structure by coupling a cellular automaton (CA) technique for grain growth with a finite element (FE) solver for heat flow (CA-FE). The advantages of the CA-FE model were that the individual grains were identified and the distribution in their shape and size was calculated, rather than just their average behavior. The model was applied to simulate CET. Since experimental data is not available for the nucleation of grains, fitted nucleation parameters were used and the results agreed reasonably with experimental observations for Al–Si alloys. In 2002, Vandyoussefi and Greer [9] applied the CA-FE model to study the effects of adding grain refiner on the as-cast grain structure in Al–Mg alloys, in particular on CET. Their results exhibited similarities with those predicted by Hunt [1]. However, the CA-FE model was based on the assumption that the envelope of the growing grains could be approximated as an ideal array of primary dendrites, i.e., the analytical solution of Kurz et al. [10] (KGT model) was assumed to relate growth velocity to tip undercooling. Using the KGT model allowed only the thermal field to be solved. However, it did not account for the solute interactions between grains or between non-ideally spaced dendrites within a grain. As will be illustrated later, omitting the effects of constitutional undercooling in these regions can significantly alter the activation potential calculated for heterogeneous nuclei located there.