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# Full length article

# Liquid channel segregation and morphology and their relation with hot cracking susceptibility during columnar growth in binary alloys



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#### ABSTRACT

The segregation and morphology of liquid channels at the last stage of solidification are closely related to hot cracking formation. We use Phase-Field (PF) simulations to investigate liquid channel characteristics during columnar growth of single-crystal and bi-crystal Al-Cu alloys. It is found that the back-diffusion is weak in Al-Cu alloys. Liquid channels in Al-2.0, 3.0 wt%Cu alloys coalesce into droplets above the eutectic temperature while the reduced Hot Cracking Susceptibility of Al-4.0 wt%Cu can be correlated to eutectic formation at the root of liquid channels. For bi-crystal growth, we demonstrate that non-equilibrium solute segregation at intergranular liquid channels (prospective Grain Boundaries (GBs)) depends on the convergent/divergent growth conditions between grains, and their misorientation angle. Divergent growth leads to stronger solute segregation as more solute diffuses laterally into divergent intergranular channels. It is thus expected that for the same GB energy, intergranular channels with higher solute composition can extend to lower temperatures, thus promote hot cracking. We introduce an approach for combining solid fraction vs. temperature curves calculated from microstructurally complex PF simulations with hot cracking models in the literature to predict the nominal composition with the highest HCS. Preliminary results from this work agrees well with experiments.

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### 1. Introduction

During columnar cellular/dendritic growth, the region where liquid and solid phases coexist due to segregation is termed as the mushy zone [1]. At the later stages of solidification, the microstructure forming inside the mushy zone is characterized by a dendritic solid skeleton with discontinuous liquid droplets and/or continuous channels distributed inside it. The liquid droplet and channels have quite different effects on the mechanical properties and hot cracking formation in the mushy zone. A solid network with liquid droplets behaves similarly to a coherent solid with slightly reduced strength and thus has a very low hot cracking susceptibility (HCS). A mushy zone with wide liquid channels can avoid hot cracking by adjusting its morphology by liquid feeding. However, when the last liquid that exists is in the form of very thin liquid channels, an opening in the mushy zone cannot generally be

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compensated by liquid feeding, and hot cracking occurs [2]. It can be concluded that the liquid channel morphology at the last stage of solidification, especially thin regions at the roots of liquid channels and grain boundaries (GBs) is critical to hot cracking.

An extensive body of experimental work has shown that the HCS of an alloy strongly depends on its nominal composition, which exhibits the typical  $\Lambda$ -shape [2,3]. The composition-dependent solidification interval (equilibrium or non-equilibrium) provides a convenient index to quantify HCS behaviour. Specifically, the larger the solidification range, the longer the liquid channel and the higher tendency of cracking. In the case of k < 1, where k is equilibrium partition coefficient, the solidification interval increases with the nominal composition initially and decreases after the formation of eutectics. The maximum freezing range thus corresponds approximately to the composition at which eutectics start to form. It is noted, however, that while eutectic reactions can take place in small liquid drops and liquid channels, it is the latter that are typically considered to have a strong effect on hot cracking formation.

Fig. 1 illustrates the trends on liquid channel morphology as a function of composition. For a dilute alloy containing only primary phase, solute segregation is weak and short liquid channels form

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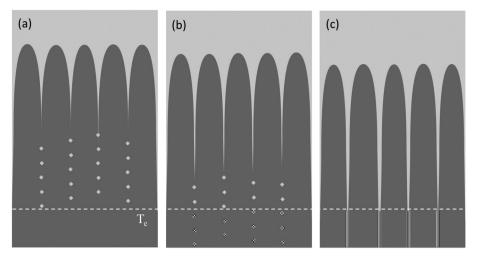


Fig. 1. Schematic diagram illustrating the effect of nominal composition on liquid channels of alloys with (a) low, (b) moderate, and (c) high concentration.

(case a). Increasing the composition to a moderate value leads to stronger segregation and longer liquid channels, with eutectic forming in isolated droplets (case b). Further increasing the nominal composition increases solute segregation further, leading to eutectic formation starting at the root of liquid channels (case c). Eutectic forming between two columnar dendrites (case c) is expected to prevent them from closing in on each other, leaving wider liquid channels that can facilitate liquid feeding and thus reduce the HCS. The distribution of metastable liquid below the eutectic temperature  $(T_e)$  is thus important to study in order to better understand hot cracking.

Normally, the length of liquid channels between the cells/dendrites can be characterized by the volume fraction of solid phase,  $f_s(T)$ , which in mean field theories is typically calculated by the Scheil equation. Here  $f_s$  is the volume fraction of solid phase and T is temperature. However, the Scheil equation can only examine volume fraction and not where dendrites coalesce. For this reason, coalescence is defined empirically to occur at  $f_s = 0.94$  and the length of the liquid is usually determined to end at this point. The real image of where the columnar dendrites join each other is still poorly understood, particularly if the coalescence point is higher or lower than the eutectic temperature. Thus, a quantitative study that includes microstructural details about dendritic coalescence is important to show a real  $\Lambda$  relationship for HCS. The importance of a precise  $f_s(T)$  predictor lies in that it is an input into models for predicating HCS, such as RDG model (Rappaz-Drezet-Gremaud).

In addition to the composition, another factor that can affect the length of liquid channel is grain boundary angle. As discussed by Rappaz [4] the grain boundary can vary from attractive to repulsive with the variation of misorientation angle. A repulsive grain boundary [4] is believed to be a necessary condition to induce hot cracking by extending the intergranular liquid channel to temperatures lower than the coalescence temperature inside a single grain,  $T_b$ . In addition to the GB energy, non-equilibrium solute enrichment can also affect liquid channels and emerging GB structures. Namely, higher solute content leads to liquid channels that extend to lower temperatures, for a fixed GB misorientation energy, and thus have a higher HCS. Luo et al. [5,6] have shown that solute segregation can make a material brittle by forming intergranular liquid channels. The role of GB energy and GB solute enrichment is convolved in alloys. To identify the effect of solute segregation alone, it would be instructive to examine large misorientation angles for which GB energy is approximately constant. It is generally expected that divergent and convergent growth will give different levels of non-equilibrium segregation at intergranular channels and resultant GBs.

Non-equilibrium morphological and segregation details inside the mushy zone and at GBs are thus quite important in providing an accurate  $f_s(T)$  for the analysis of hot cracking formation. The Phase-Field (PF) method, with the advantage of avoiding interface tracking, has been widely used to modelling microstructure development [4,7–10]. In addition, with the advent of accessible thin interface limit analyses coupled to parallel adaptive mesh refinement codes, the PF method has become a viable tool for handling large-scale simulations that can examine the development of the mushy zone in experimentally relevant systems for both single or polycrystalline columnar growth.

Using the Multi-Phase Field modelling approach, Böttger et al. have examined microstructure formation and its relationship with HCS during continuous casting of polycrystalline Low-Carbon and High-Strength Low-Alloyed Steels [11–13]. Their simulations show that micro-alloying such as Ti and related precipitates have a pronounced effect on HCS by increasing the coalescence temperature.

This work uses a recent quantitative Multi-Order Parameter phase field model of alloy solidification to study HCS in solidification under laser welding conditions in the Al-Cu system, with the aim of isolating and characterizing the specific roles of solute on coalescence and eutectic formation in single crystal and bi-crystal columnar growth, as well as non-equilibrium segregation effects on the coalescence of bi-crystal grain boundaries. In the case of single crystal directional solidification, the effect of the nominal composition on liquid channel segregation and morphology is examined, and the results using the Scheil equation are compared to from PF simulations. In the case of bi-crystal directional solidification, the dependence of intergranular solute enrichment on convergent/divergent growth conditions and mis-orientation angle are characterized. Finally, we also couple analysis from our phase field simulations to the RDG and Kou models of hot cracking to specifically identify the nominal composition corresponding to the highest HCS in Al-Cu alloys. Our results demonstrate that the effect of the nominal composition, divergent/convergent growth conditions and misorientation angle between bi-crystals, can have a significant effect on solute segregation and, thus, hot cracking formation in welding processes.

## 2. Phase field model of polycrystalline solidification

To investigate solute segregation at liquid channels and

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