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Characterization of late-stage equiaxed solidification of alloys

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Abstract

We use a two-dimensional phase-field model coupled to a nucleation mechanism to study the evolution of interdendritic liquid pools during late-stage solidification of Mg–Al alloys under spatially uniform temperature and constant cooling rates. We obtain the channel size distribution (CSD) of liquid pools at solid fractions close to those where eutectic phase is expected to form and investigate the influence of cooling rate on the morphology of the CSD at different solidification stages. Our results show that the CSD is unimodal, exhibiting a peak at small channel widths followed by a shoulder and longer decay tail at large channel widths. This feature is correlated to the presence of two distinct liquid regions, small channels between secondary branches of the primary phase and larger channels between adjacent grains. We construct a cooling-rate/solid-fraction morphology diagram that shows the relative importance of the shoulder in the CSD. We characterize the mean and standard deviation of the CSD and show that, within the range of data examined, the mean channel size vs. cooling rate curves scale with solid fraction. The numerical tools developed for this work can also be used to analyze experimental results. We include the analysis of two experimental micrographs previously published by Paliwal et al.

Keywords: Phase-field model; Solidification microstructure; Binary alloys; Dendritic growth

1. Introduction

The as-cast microstructure as well as the spatial distribution of solutes that develops during the primary phase of solidification serves as a template for the formation of secondary phases in metal alloys. There has been extensive research on microstructure selection of primary phases during solidification in alloys [1–9] using dynamical experiments and phase-field simulations. The selection of secondary phases is typically predicted by applying thermodynamic models of equilibrium phases to the thermosolutal conditions during late-stage solidification [10,11]. However, to date most such studies usually ignore the role of complex interface topology and liquid pool confinement on the second-phase selection process.

Numerical modeling has become rapid and sophisticated enough to simulate the evolution of very complex interface topologies during solidification, topologies that would otherwise be difficult to observe experimentally, and which can help clarify the mechanisms by which the final properties of alloy phases emerge. For example, using multicomponent and multiphase field models [12–14], it is possible to characterize and measure the distributions of multiple solutes and correlate them to the morphology of liquid channels that form between primary phases throughout the solidification path. By studying interdendritic liquid pools at the stage at which they become precursors of

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secondary phases, it is thus possible to gain insights into the final distribution and type of second phases of the resulting alloy.

In this work we model the liquid pool evolution in the late stages of solidification of a binary alloy of composition Mg–10 wt.%Al under conditions of uniform temperature and constant cooling rate. The aforementioned composition is chosen due to its similarity to AZ91 Mg alloy, which is a well-known commercial alloy the properties of which have been extensively studied [16–19]. Fig. 1 shows two experimental micrographs of Mg–9 wt.%Al for different cooling rates: 30 and 75 K s^{-1} [15]. In both cases the microstructure consists of a convoluted network of narrow second-phase channels between grains of primary phase, a morphology that is typical of dendritic growth. In order to characterize such microstructure, we calculate the channel size distribution (CSD) of the interdendritic liquid channels at solid fractions close to those at which they would become precursors of eutectic phase. The mean channel width, its standard deviation and the structure of the CSD distribution are examined as a function of primary solid fraction and cooling rate. Making the reasonable assumption that the transformation of supersaturated liquid pools into eutectic occurs at much shorter timescales than those that characterize primary phase evolution,[1] we may regard the results of this study as defining a statistical metric for characterizing the distribution of secondary phases. A future publication will address the question of how secondary phases emerge from the liquid during late-stage solidification.

The structure of this paper is as follows. Section 2 introduces the methods we use to simulate the microstructure and solute concentration dynamics, as well as to obtain the CSD. In Section 3 we present and discuss our results regarding the characterization and scaling of interdendritic liquid pools. Finally, in Section 4 we present our conclusions and an outlook on future work.

2. Methods

2.1. Nucleation algorithm

We coupled our phase-field model solidification process to a quantitatively accurate model for nucleation in order to obtain a realistic spatial distribution of grains as well as the undercooling at which they appear. Our model considers heterogeneous nucleation on inoculant particles as the sole mechanism of grain inception. We follow the stochastic coarse graining approach of Simmons et al. [20], already applied successfully in Ref. [21] to a binary alloy. This approach consists of calculating the probability of spontaneous nuclei formation within a certain volume element during a certain time interval. The following

[1] An argument in support of this hypothesis is presented in the discussion of Fig. 4 in Section 3.2.

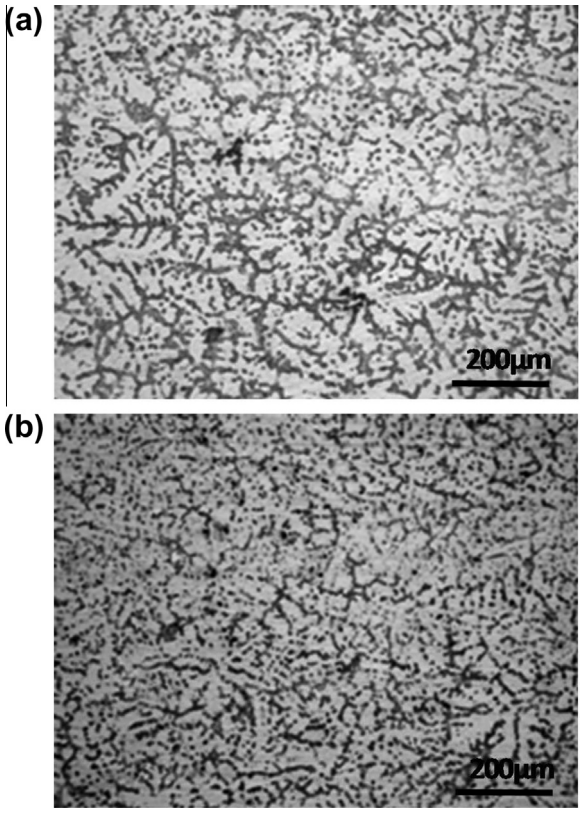

Fig. 1. Optical micrographs of Mg–9 wt.%Al under cooling rates (a) 30 K s^{-1} and (b) 75 K s^{-1}. Reprinted from [15] with permission.

expression yields the probability p_N that at least one solid nucleus of critical size forms within a homogeneous volume element ΔV during a time interval Δt:

$$p_N = 1 - \exp(-J\Delta V\Delta t), \quad (1)$$

where J is the nucleation rate which depends on the local conditions of the metastable liquid, the physical properties of the material, and the nature and concentration of inoculant particles. The coupling of nucleation to phase-field dynamics that simulate dendritic growth is described in more detail in Ref. [21].

2.2. Phase-field model

We use a phase-field model to simulate growth after nucleation of equiaxed grains of Mg–10 wt.%Al. This model is a modified version of the quantitative phase-field model for dilute binary alloys described in detail in Ref. [22], and further extended for general two-phase polycrystalline binary alloys [23] by Ofori-Opoku et al. [24]. Our model includes thermal noise to promote sidebranching. Details on the inclusion of thermal noise in the model can be found in Refs. [7,25]. We also include non-vanishing, temperature-dependent solute diffusivity in the solid which is responsible for back-diffusion. For the range of temperatures considered, the solute diffusivity varies within two orders of magnitude. The evolution of solidifying domains of primary phase is found by numerical