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Quantification and classification of microstructures in ternary eutectic alloys using 2-point spatial correlations and principal component analyses

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ABSTRACT

Eutectic solidification gives rise to a number of distinct microstructure patterns that might include lamella, rods and labyrinths in binary alloys. However, as the number of phases and components increases, the number of possible patterns that might be obtained during bulk solidification also become larger. While the morphological attributes of binary eutectic solidification have been fairly well understood, the same is not true for ternary and higher multicomponent alloys. In this paper, we study and quantify microstructures in ternary alloys as a function of two essential parameters, namely, the volume fraction of the solid phases and the surface energies of the interfaces (in particular the solid–liquid interfaces). For the selected ensemble of microstructures, quantification and classification were carried out using a recently developed data-driven (objective) approach based on principal component analyses of 2-point correlations. It is demonstrated that the method is capable of analyzing and quantifying the similarity/difference measures between the elements of the selected ensemble of microstructures.

1. Introduction

Three-phase, ternary eutectic growth has been a topic of high interest for both experimentalists as well as theoreticians owing to the rich variety of patterns or microstructures possible. Rigorous study of these microstructures can provide an improved understanding of the principle mechanisms of general importance for the development of multicomponent alloys needed in advanced technology applications. Experimental investigations of ternary alloys have been carried out for both metallic [1] and inorganic alloys [2] for thin-film solidification conditions. Bulk solidification of three-phase growth has also been studied extensively [3–9]. However, theoretical investigations of three-phase growth have been few. Himemiya and Umeda [10] have worked out analytical expressions for undercooling as a function of spacings for different three-phase configurations. Modeling efforts for thin-film and bulk solidification patterns were described in a few papers [11,12].

One of the widely studied alloys in this regard is the Ag–Al–Cu alloy [13–18] which classically shows patterns of the type as shown in Fig. 1(a). However, there are other systems such as the Nb–Al–Ni ternary eutectic system [19] that exhibit quite different patterns compared to those seen in the Ag–Al–Cu alloy. These observations raise interesting questions regarding the correlation of microstructure features to material and/or processing parameters.

In recent work [21], a phase-field simulation study was performed to understand how surface energies and volume fractions influenced the microstructure pattern formation during three dimensional directional solidification. For this purpose, the authors started with a symmetric model ternary eutectic alloy with equal surface energies, and investigated the individual influence of volume fractions and surface energies. For the study on the influence of volume fractions, continuous simulations were performed along the two composition pathways shown in Fig.2. In this set of simulations, the composition of the far-field liquid was changed periodically after sufficient time-intervals, during which the pattern at a given composition of the liquid is allowed to get reasonably close to the steady-state condition.

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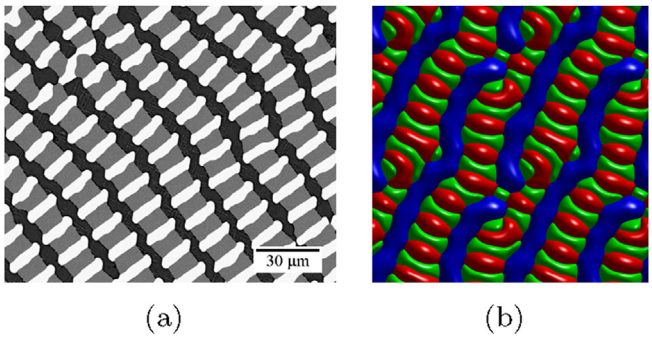

Fig. 1. In (a) a typical microstructures in a directionally solidified Ag–Al–Cu ternary eutectic alloy [20], white: Ag_2Al, grey: Al_2Cu, black: Al. In (b) a phase-field simulation of the same system showing similar morphological characteristics as in the experiment, but with different ordering of the phases. Blue: Al_2Cu, green: Ag_2Al, red: Al. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

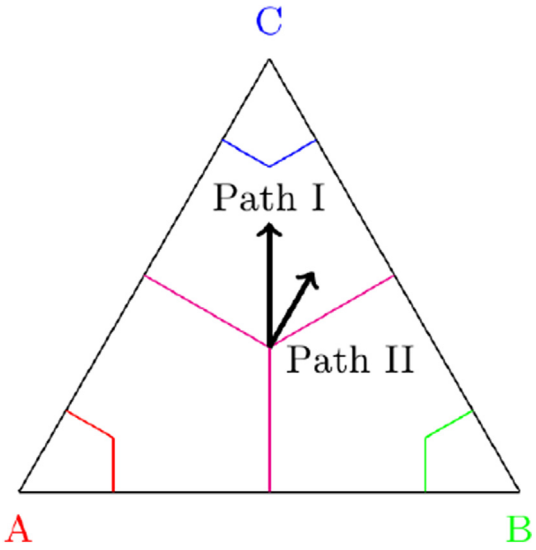

Fig. 2. Schematic of the liqiudus projections (magenta) and solidus projections of the three solid phases, along with the two composition pathways for which the simulations were performed. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Thereafter, two simulations were performed to investigate the influence of solid–liquid interfacial energies both independently and in combination with change in volume fractions. Additionally, some insights into pattern formation of real alloys were also derived from phase-field simulations coupled with thermodynamic databases. From these, it was possible to derive structures displayed in Fig.1(b), which resemble the experimental structures highlighted in Fig.1(a).

While, the simulation study was able to span a wide range of volume fractions, solid–liquid surface energies and also a different phase diagram, the study remains qualitative in terms of quantifying the different structures obtained. Also, there is a critical need to extend the study to include different combinations of the solid–solid surface energies.

In this work, we draw upon the simulation results from the previous work referenced above [21], and add critical missing microstructures; this completes the ensemble of microstructures depicting the wide variety of possibilities of structure formation in three-phase systems. Thereafter, we present an analysis of some of the geometrical features that exhibit the highest sensitivity to changes in the volume fractions. As we will see, a change in the processing conditions or the processing parameters brings upon changes in multiple features in the microstructure. As a result, it often becomes difficult to identify or extract a precise correlation between the process parameters and the predicted microstructure. In this paper, we have therefore decided to explore these correlations using a much more objective and quantitative framework. This recently formulated framework employs two-point spatial correlations to rigorously quantify the material microstructure in a statistical framework. The method subsequently employs principal component analysis (PCA) to obtain an objective low-dimensional representation of the material microstructure. Since PCA accomplishes the dimensionality reduction in ways that maximizes the capture of the variance between the elements of the dataset in the minimum number of terms, it is ideally suited for our purpose. The PC representations are then used to quantify the magnitude of resemblance/differences between the different microstructures obtained in the simulation study.

2. Brief summary of the simulation results

2.1. Microstructures from prior work

In this section, we recall the simulation results from Ref. [21], as they will be included in the statistical analysis conducted in this study. For the purely symmetric ternary eutectic phase-diagram, with equal surface energies for all interfaces, the phase-field simulations give rise to a mostly regular polygonal structure of the form highlighted in Fig. 3.

Figs. 4 and 5 represent simulated microstructures along Path I and Path II, respectively, as described in Fig.2 (cf. [21]). An interesting question one could ask is: what would happen, if we were to take back the composition to the ternary eutectic point. To address this, we directly ramped up the far-field composition from the final state in Fig. 5(f), and were able to get to the complete hexagonal state, with a regular-brick structure in the intermediate evolution, Fig.6.

In order to access the influence of surface energies we performed calculations wherein, the solid–liquid interfacial energies

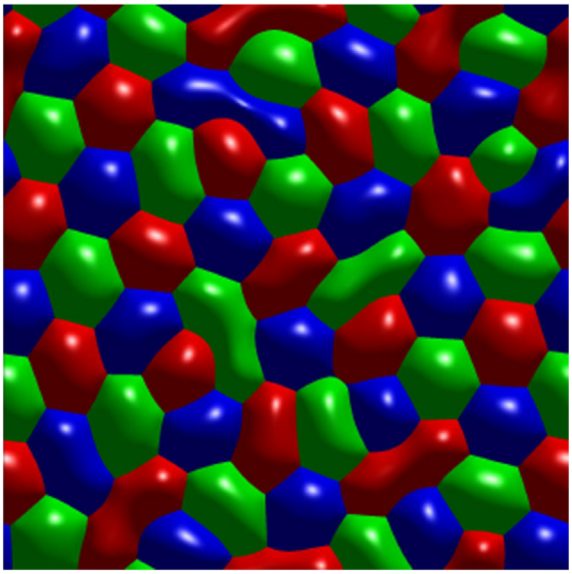

Fig. 3. Phase-field simulation of purely symmetric ternary eutectic system at the eutectic composition.