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Study of pattern selection in 3D phase-field simulations during the directional solidification of ternary eutectic Al-Ag-Cu

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ABSTRACT

During the directional solidification of ternary eutectic alloys, different arrangements of the three solid phases evolve, leading to multiple microstructure patterns. These patterns influence the macroscopic properties of the alloy. Different arrangements are even found in single micrographs for the same imposed process conditions. Gaining a better understanding of the complex mechanisms leading to these different patterns is crucial to obtain tailored microstructures with specific properties. To exploit the different patterns which appear in ternary eutectic Al-Ag-Cu, a coupled approach is undertaken using a large-scale simulation and extensive parameter studies on smaller 3D domains. Three patterns found in both large-scale simulations as well as experimental micrographs are investigated with smaller domain size simulations by systematically varying the lamellar spacings. The resulting undercooling-spacing correlations of all investigated phase arrangements follow a Jackson-Hunt-type shape. Different stability ranges of the initially set microstructure are found, and depending on the lamellar spacings, the pattern with the lowest undercooling changes. The combination of both outcomes gives an explanation for the presence of different patterns within single micrographs of directionally solidified ternary eutectic alloys.

1. Introduction

The casting of metallic alloys is one of the most important industrial manufacturing processes [1]. The evolving microstructure during solidification influences the resulting macroscopic material properties [2–4]. For example, the average grain size is directly related to the yield stress as described by the Hall-Petch relation [5,6]. During the directional solidification of alloys with a eutectic composition, an in situ composite material evolves [7]. With this kind of casting process the size of the evolving rods and lamellae in the microstructure [8] can be controlled by the solidification velocity. The correlation between the solidification velocity, the size of the evolving microstructure, and the resulting undercooling at the solid–liquid interface is analytically described by Jackson and Hunt [9] for directionally solidified binary eutectics in 2D.

In ternary eutectic alloys, the evolving phases arrange in various patterns in the microstructure [10–14]. Besides the size, the type of evolving patterns also influences the macroscopic material properties [15]. For ternary eutectic alloys, five idealized patterns are predicted from geometrical considerations in [16,17]. Analytically, eight different patterns are studied in [18–21]. However, the microstructures which arise in experimental cross sections are more complex [11–14,22,23] than theoretically and analytically predicted microstructures. Depending on the process conditions, six different patterns are found in micrographs parallel to the solidification front of ternary eutectic Al-Ag-Cu in [22]. Furthermore, for this system multiple patterns are observed in a single micrograph as exemplarily shown in Fig. 1. This micrograph shows simultaneously evolved chain-like structures in the lower right and paw-structures in the upper left part. The sample [24] solidified with a velocity of 0.32 µm/s and a temperature gradient of 2.8 K/mm in the Artemis facility [25].

A better understanding of the mechanisms leading to different patterns is required to produce tailored microstructures with defined patterns. Therefore, in this work the correlation between process conditions and the evolving patterns is studied with phase-field simulations. The phase-field method has been established in recent years as a versatile and powerful tool to investigate the microstructure evolution during solidification [26–31]. Studies

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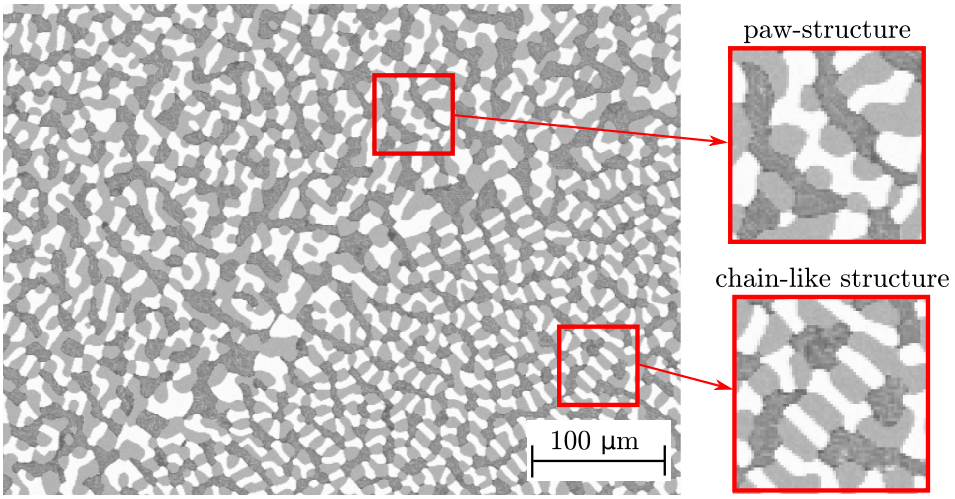

Fig. 1. Experimental micrograph of directionally solidified ternary eutectic Al-Ag-Cu parallel to the growth front from Dr. A. Dennstedt [24]. The sample solidified with a velocity of 0.32 µm/s and a temperature gradient of 2.8 K/mm in the Artemis facility [25]. In the lower right part, a chain-like structure of the two intermetallic phases Ag_2Al and Al_2Cu embedded in an Al-matrix is detected. In the upper left part, less well aligned paw-structures evolved simultaneously for the same imposed process conditions.

of ternary eutectic Al-Ag-Cu systems with the phase-field method are published in [8,32–39]. The occurrence of different patterns resulting from varying melt compositions and growth velocities is studied in [34] and in [8], respectively.

For the correlation between solidification velocity, lamellar spacings and the resulting undercooling, a good quantitative accordance between phase-field simulations and an analytical approach is found in [20] for two-dimensional idealized ternary eutectics. It is demonstrated, that depending on the 2D lamellar arrangements, different average front undercoolings adjust.

For three-dimensional ternary eutectic microstructures, the interplay between the adjusting front undercooling and the arising patterns at different lamellar spacings is not yet fully understood. Hence, the purpose of this work is to study the undercoolings of different 3D patterns and to identify their stability ranges. With these, predictions of the preferred pattern for certain lamellar spacings can be given.

To investigate the free pattern evolution in a representative volume element [35], a large-scale simulation with a domain size of $4116 \times 4088 \times 4325$ voxel cells corresponding to approximately $1.6\ \text{mm} \times 1.6\ \text{mm} \times 1.7\ \text{mm}$ is conducted. The patterns arising in this simulation are studied in detail using multiple smaller simulations each exhibiting a unique pattern. In these extensive 3D simulation studies, the lamellar spacings are systematically varied and the resulting undercoolings are determined.

For this study, first the applied phase-field model and simulation setup is presented. Then the results from the large-scale simulation are shown. Based on these results, three patterns observed in the large-scale simulation that correspond to patterns observed in experimental micrographs of Al-Ag-Cu are studied. Finally, the findings are compared and discussed, and the conclusions of this work are presented. The results of this work are a continuation of the outcomes presented in [39].

2. Phase-field model

To investigate the microstructure arrangement of multiple patterns and their evolving undercoolings, a thermodynamically consistent phase-field model based on the grand potential approach [31,40] is used. A detailed description of the model is presented in [32] and its validations in [21,35,32,39]. The solidification process is modeled by solving a coupled set of four phase-field equations (three solid phases and the melt) and three chemical potential evolution equations in a ternary system. The growth direction and velocity v is controlled by a moving analytical temperature field. The model is discretized with finite differences in space and an explicit Euler scheme in time as given in [41]. The implementation of the model is a combined solution of the PACE3D package [42] and the massive parallel framework WALBERLA[1] [33,43]. Simulation results with this model for idealized systems are presented in [44] and for realistic eutectic systems in [8,34,45–47].

3. Simulation setup

For the simulations the setup depicted in Fig. 2 is used to describe a solidification in a Bridgman-type furnace. To model an infinite domain, periodic boundary conditions perpendicular to the solidification front are applied. Parallel to the solidification front, a Dirichlet boundary condition is used at the liquid side and a Neumann boundary condition is employed on the solid side. To study the influence of different lamellar spacings on the evolving undercooling, the plane parallel to the growth front is systematically varied. This plane is called base size in accordance with [44] and is depicted as a red plane in Fig. 2.

For studying free pattern formation unconstrained by the boundary conditions a large-scale simulation with a base size of more than 4000×4000 voxel cells is conducted. As initial microstructure a Voronoi tessellation similar to Fig. 2(a) with nuclei multiple times smaller than the evolving rods is used. For the studies in this work the ternary eutectic system Al-Ag-Cu with the parameters given in [8,32–34,38,39] is applied. The conversion factors to physical units are given in [32]. In the ternary eutectic system Al-Ag-Cu the solubility of Ag in the Al-phase changes strongly after the solidification, leading to different phase fractions at room temperature [11,48,49]. To mimic the phase fractions observed in experimental samples after the solubility shift [10–13,50], in all simulations of this work an adjusted system is applied. The ternary eutectic point is shifted to 0.237 mol% Ag, 0.622 mol% Al and 0.141 mol% Cu. This adjusted system is also used in [8,32–35,38,39,51].

To improve the computational efficiency and to increase the convergence rate of the average front undercooling during

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