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Branching-induced grain boundary evolution during directional solidification of columnar dendritic grains

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A B S T R A C T

We present an investigation of secondary and tertiary branching behavior in diverging grain boundaries (GBs) between two columnar dendritic grains with different crystallographic orientations, both by two-dimensional phase-field simulations and thin-sample experiments. The stochasticity of the GB trajectories and the statistically averaged GB orientations were analyzed in detail. The side-branching dynamics and subsequent branch competition behaviors found in the simulations agreed well with the experimental results. When the orientations of two grains are given, the experimental results indicated that the average GB orientation was independent of the pulling velocity in the dendritic growth regime. The simulation and experimental results, as well as the results reported in the literature exhibit a uniform relation between the percentage of the whole gap region occupied by the favorably oriented grain and the difference in the absolute values of the secondary arm growth directions of the two competitive grains. By describing such a uniform relation with a simple fitting equation, we proposed a simple analytical model for the GB orientation at diverging GBs, which gives a more accurate description of GB orientation selection than the existing models.

1. Introduction

During many casting processes, columnar grains consisting of packages of dendrites are formed following the initial formation of fine equiaxed grains near the surface; preferred orientation is then produced through the competitive growth of columnar dendritic grains. In 1959, Walton and Chalmers [1] first proposed a selection mechanism for the competitive grain growth based on the difference in tip undercooling of unfavorably oriented (UO) and favorably oriented (FO) dendrites. UO dendrites, also called misoriented dendrites, grow at relatively larger angles with respect to the thermal gradient than FO dendrites or well-oriented dendrites. It was recognized that the tip undercooling of the UO dendrites should be higher than that of the FO dendrites, i.e., the tips of UO dendrites lag behind those of FO dendrites. This lag in dendrite tips leads to overgrowth of UO grains. Because this selection mechanism seemed to agree well with some early experiments [2,3], the criterion according to the magnitude of dendrite tip undercooling has been widely used to determine the outcome of competitive grain growth. It is usually thought that a grain consisting of more misoriented dendrites will be eliminated faster owing to the higher dendrite tip undercooling. However, recently, a series of experimental [4–10] and numerical studies [11–16] on directional solidification have challenged this traditional viewpoint. It has been found that although the dendrites in UO grains exhibit higher undercooling than those in FO grains, the UO grains may survive longer than expected or even continuously grow larger [4,5,11,14–16], whereas FO grains may be eliminated by their UO neighbors [6–10,12–16]. These unusual grain selection phenomena indicate that the difference in dendrite tip undercooling is not always suitable for predicting the outcome of competitive grain growth.

The selection of columnar dendritic grains is directly determined by the migrations of grain boundaries (GBs). In two dimensions, a grain with GBs on both sides migrating away from each other will dilate, whereas one with GBs migrating toward each other will shrink. Thus, the unusual grain selections found in recent studies [6–10,12–16] are due to unexpected GB evolution behaviors, which are different from the usually accepted model [1]. The quantitative prediction of competitive grain growth requires a

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comprehensive understanding of the relations between the GB orientation and control parameters such as the orientations of the two grains forming the GB, pulling velocity, and temperature gradient. However, the establishment of such relations is still far from satisfactory.

Bi-crystal competition is usually divided into two types according to the relative growth direction of the two grains: converging growth and diverging growth, as schematically shown in Fig. 1(a1)–(a3) and (b1)–(b3). The GBs corresponding to the two cases are referred to as converging GBs and diverging GBs, respectively. The evolution of converging GBs is governed by blocking of the primary dendritic arms. Because the UO dendrites lay behind the FO dendrites, as suggested by the Walton and Chalmers model, it is usually assumed that the UO dendrites should be always blocked by their FO neighbors, which means the orientations of converging GBs should follow the growth direction of the FO dendrite. However, the so-called "unusual overgrowth," i.e., the overgrowth of FO dendrites by UO dendrites at the converging GB, has been recently confirmed both by experiments [6,7] and phase-field simulations [12,13]. This unusual overgrowth inclines the GB toward the FO grain. The mechanism of this phenomenon has been revealed by the present authors [12] and by Takaki et al. [13]. Further, Tourret and coworkers [16] ascertained the range of bi-crystal orientation for the occurrence of unusual overgrowth in the 2D dendritic growth regime, and they proposed a simple linear interpolation formula to calculate the GB orientation when such unusual overgrowth occurs.

As compared to the considerable progress in converging GB orientation selection, the present understanding of diverging GB orientation selection is still limited. The evolution of diverging GBs is determined by a new primary arm generation through tertiary branching in the spatially extended gap between two grains. According to the proposal by Walton and Chalmers [1] and the schematic illustration of Rappaz and Gandin [2], a new primary arm can form from both the FO grain and the UO grain, which means that the orientation of the GBs should lie between the dendritic growth directions of the FO and UO grains. However, a quantitative relation between the GB orientation and the two growth directions is unclear. Some studies have been carried out to establish such a relation. Based on the experimental results of a transparent alloy in a thin sample, Esaka and coworkers [17,18] assumed that the GB bisected the two growth directions in all diverging configurations. Within bi-crystal volume samples illustrating a configuration similar to that shown in Fig. 1(b1), Zhou et al. [6] found that when the misorientation of the UO grain is less than 20°, the GB angle increases linearly with the difference in misorientation of the two competing grains. Recently, using phase-field simulations, Tourret and Karma [15,16] showed that the selection of a diverging GB trajectory is stochastic because of the inherent stochasticity of side branching and the subsequently chaotic dynamics of branch

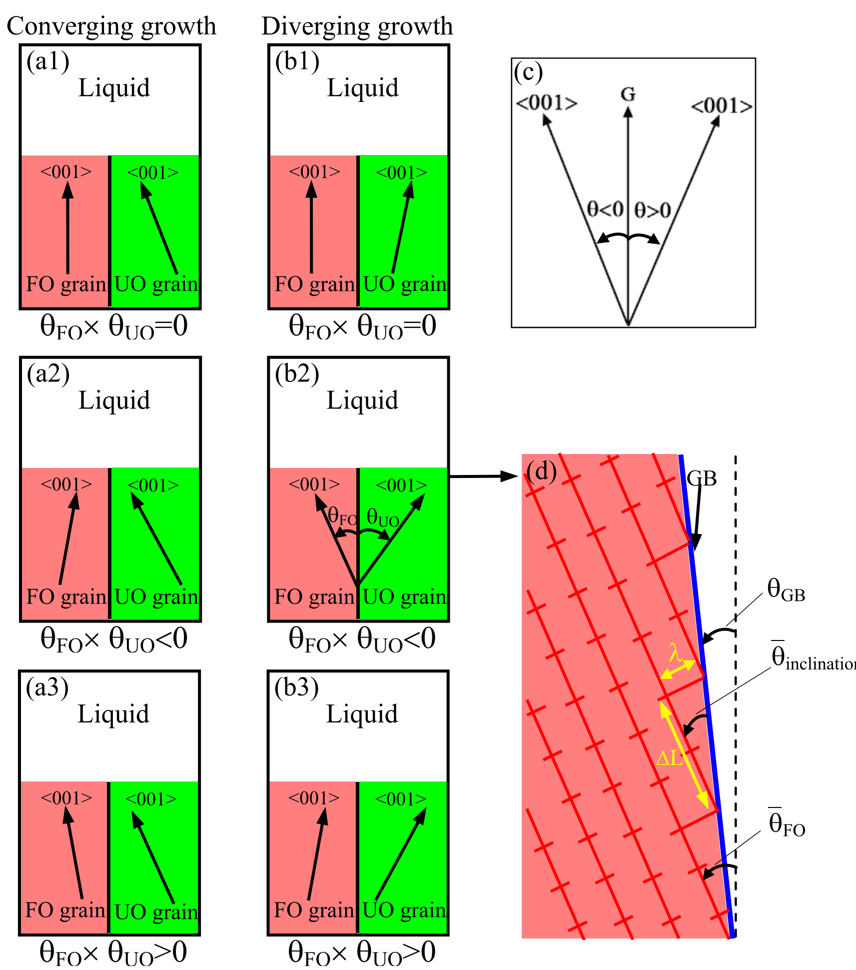

Fig. 1. Schematics of bi-crystal configurations in which the crystal orientations of the two grains (a1)–(a3) result in converging dendritic growth and in (b1)–(b3) diverging dendritic growth. (c) Angles defined clockwise with respect to the thermal gradient direction. (d) Development of a new primary arm from the FO grain inclines the GB from the growth direction of the FO grain.