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# Non-uniplanar competitive growth of columnar dendritic grains during directional solidification in quasi-2D and 3D configurations

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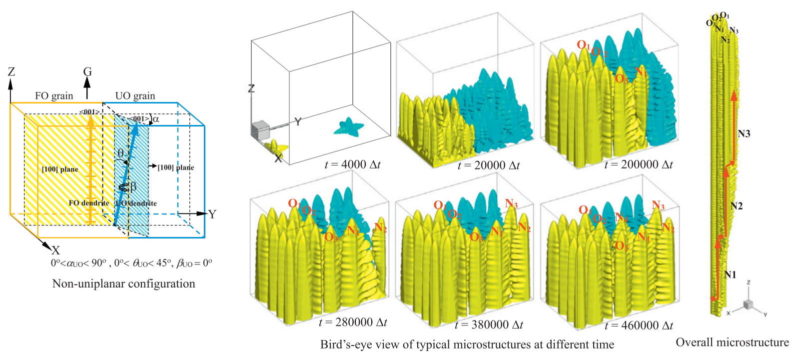
## HIGHLIGHTS

- Phase-field simulations were extended to the more common bicrystal configurations with non-uniplanar dendrite growth directions.
- The grain boundary motion behavior was observed during non-uniplanar competitive growth in three-dimensions.
- The overgrowth rates of two-dimensional diverging growth and three-dimensional non-uniplanar competitive growth were compared to illustrate the difference between the two cases.

## GRAPHICAL ABSTRACT

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## ABSTRACT

The competitive growth of bicrystals during directional solidification in both thin samples and three-dimensions (3D) was investigated by phase-field simulations. Unlike previous studies, which assumed the <001> orientation of the two competing grains to be in the same plane or in two parallel planes which are normal to the contacting plane of two grains, simulations in the present study focused on the more common configurations in which the <001> orientation of the two grains is non-uniplanar. Simulations of competitive growth in thin samples showed that the deviation of the <001> orientation of an unfavorably orientated grain from the sample plane caused difficulty in the generation of new primary arms from the unfavorably orientated grain. Therefore, the grain boundary orientation in thin samples may deviate from that in two-dimensions (2D), even though the bicrystal configuration observed in the thin-sample plane appeared similar to that in the 2D. It was found that in 3D, the new primary arms could develop from the favorably oriented dendrites along two directions to occupy the gap left by the unfavorably orientated grains, which led to a faster overgrowth rate of the unfavorably orientated grains than that in the case of diverging growth in 2D.



## 1. Introduction

In many casting processes, columnar dendritic grains are usually formed after the formation of fine equiaxed grains on the casting surface. The competitive growth between dendrites with different orientations becomes a key factor influencing the final microstructures and mechanical properties of the cast product. Depending on the difference in the degree of deviation of the orientation from the thermal gradient, dendrites are usually classified as favorably oriented (FO) dendrites or unfavorably oriented (UO) dendrites. UO dendrites deviate from the thermal gradient direction by a larger angle than do FO dendrites. On the basis of analyses of the difference in tip undercooling between these two kinds of dendrites, Walton and Chalmers [1] proposed

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the first-ever model for competitive growth. It was recognized that the UO dendrite always lag behind the FO one due to a larger growth undercooling, which leads to the elimination of the UO grain. Although some experimental observations [2–4] were consistent with this classical model, some inconsistent or more complex results [5–20] have also been found, such as FO dendrites may be blocked by their UO neighbors for converging growth [6–10,12–16], which is termed unusual overgrowth, and FO dendrites sometimes cannot generate new primary arms during diverging growth [5,16,17]. In recent years, detailed studies have been conducted on such differing behaviors from the prediction of the Walton–Chalmers model, especially by means of phase-field simulations [12–17].

The phase-field model is a powerful tool for modeling the evolution of microstructures during many solidification processes [21–25]. The present authors [12] and Takaki et al. [13] clarified the influence of solute interaction on the unusual overgrowth, i.e., converging growth, of columnar dendritic grains in two-dimensional (2D) directional solidification. Further, Tourret and coworkers determined the range of bicrystal orientations in which unusual overgrowth would occur [16]. Tourret and coworkers [16] established an analytical model for the selection of diverging grain boundary (GB) orientation in the case of diverging growth in 2D. However, this model makes a rough approximation in some cases of bicrystal configurations. In our recent study [17], through analyzing the simulation and experimental results, as well as the results reported in the literature, we found that the occupation of the gap region between two diverging grains by the FO grain is mainly determined by the difference in the absolute values of the secondary arm growth directions of the FO and UO grains. The results from different situations and systems 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.

Present understanding of dendrite growth competition in three-dimensions (3D) is still limited in comparison to the considerable progress made in understanding of dendrite growth competition in two-dimensions (2D). Competitive growth in 3D is more complicated than that in 2D. The grain orientation in 3D can be determined by three angles as shown in Fig. 1(a1): the rotation angle $\alpha$, which is the angle by which the [100] plane of the grain rotates about the thermal gradient direction; the inclination angle $\theta$, which is the angle by which the <001> crystal direction deviates from the thermal gradient direction; and the azimuthal angle $\beta$, which reflects the rotation of the secondary arm about the axis of the primary arm (the <001> direction). The positive values of these angles are defined as shown in Fig. 1(a1). Here, the bicrystal configurations are termed uniplanar when the primary dendrite arms of two competing grains can be in the same plane (Fig. 1(b1)) or in two parallel planes (Fig. 1(b2)), meanwhile the plane or two parallel planes containing primary arms should be normal to the contacting plane of the two grains. Otherwise the configurations are named as "non-uniplanar" just as two examples shown in Fig. 1(a1) and (a2). It should be noted that although the configuration in Fig. 1(a2) also exhibits the character that the primary dendrite arms of two grains are in two parallel planes (the [100] plane of UO grain and the [010] plane of FO grain,), these two parallel planes are parallel to the contacting plane of two grains (X-Z plane), rather than being normal to the contacting plane as the uniplanar case.

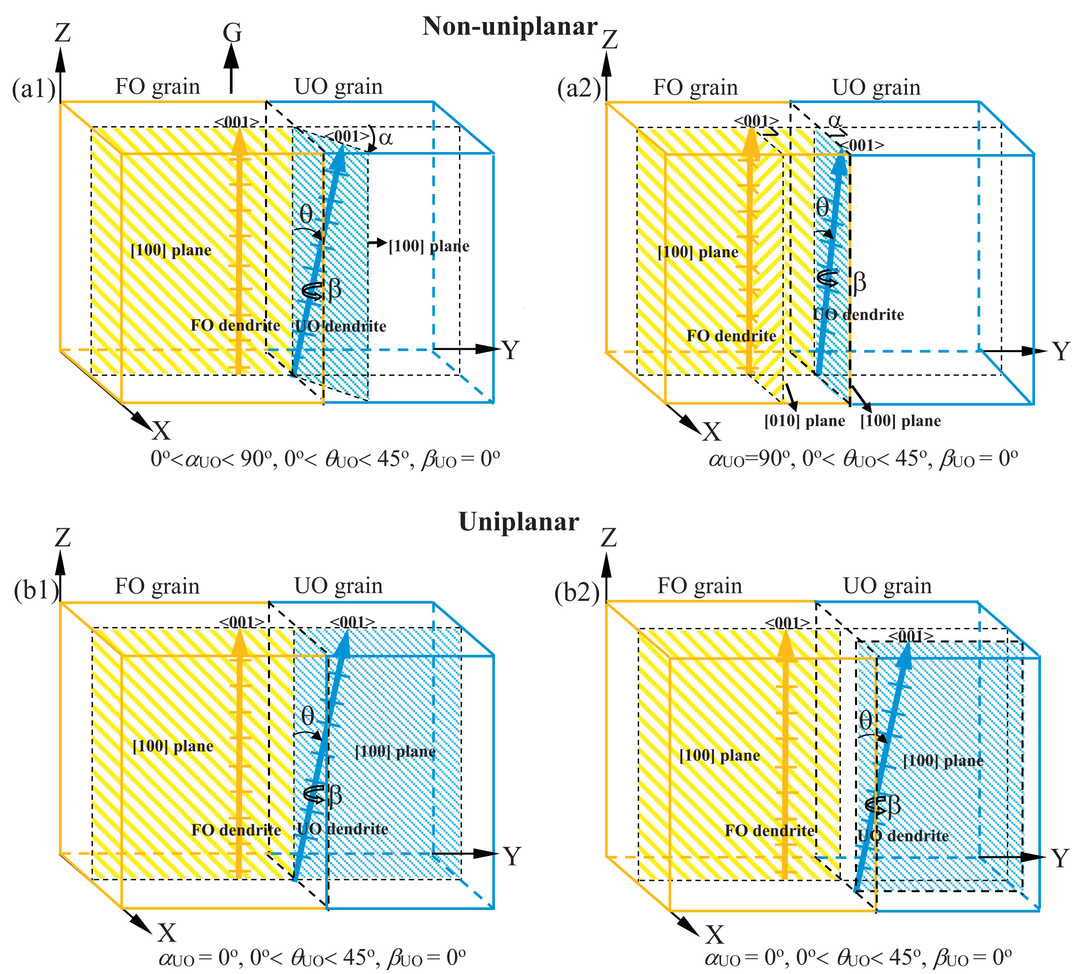


**Fig. 1.** Schematics of bicrystal orientations in 3D reference frame. (a1)–(a2) Non-uniplanar configuration and (b1)–(b2) uniplanar configuration. The definitions of the rotation angle $\alpha$, inclination angle $\theta$, and azimuthal angle $\beta$ are illustrated here.