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Phase-field modeling of twin-related faceted dendrite growth of silicon

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A R T I C L E I N F O

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We investigated the growth of a twin-related silicon dendrite through a novel phase-field model. The correctness of the model for an equilibrium twined crystal was examined first before we modeled the faceted dendrite growth. The simulated morphologies of ⟨112⟩ and ⟨110⟩ faceted dendrites were consistent with experimental observations. The growth orientation of the simulated dendrite depended on the growth rates at the ridges and the re-entrant corners. We further extended the Twin-Plane-Reentrant-Edge (TPRE) mechanism and then proposed a new growth model for faceted dendrites based on our simulations. The undercooling and twin spacing could affect the growth rates at the ridges and the re-entrant corners, which were also explained by the proposed model.

1. Introduction

Dendritic growth behaviors of semiconductors have attracted much attention due to their unique crystal morphologies. Unlike metallic dendrites, dendrites of faceted materials such as Si and Ge are often found under sufficient undercooling [1–21]. For Si or Ge dendrites, the surface of faceted dendrites is bounded by habit planes. The growth direction and morphology of a faceted dendrite also varies with undercooling. For instance, ⟨112⟩, ⟨110⟩ and ⟨100⟩ faceted dendrites have been reported in different undercooled Si [8,11–21] or Ge melts [1,2,4–6,9,10]. In particular, ⟨112⟩ and ⟨110⟩ faceted dendrites appear at ΔT (undercooling) <100 K in an undercooled Si melt [14], and more than two parallel twin planes can be found at the center of these dendrites [14,15]. The schematic diagram of growth behaviors of ⟨112⟩ and ⟨110⟩ faceted dendrites are shown in Fig. 1. In Fig. 1(a) and (b), the twin planes are in (111) orientation, while in Fig. 1(c) the twin planes are parallel to the observation direction.

Hamilton and Seidensticker [3] proposed the Twin-Plane-Reentrant-Edge (TPRE) mechanism to explain the rapid growth of twin-related faceted dendrite, as illustrated in Fig. 2(a). The nucleation event at corners with an external angle of 141° (type-1) leads to the formation of a new growth step, with the re-entrant corners of 109.5° (type-2), as indicated by 2 in the second crystal in Fig. 2(a). According to the nucleation theory, the nucleation rates at both types of re-entrant corners are in the same order of magnitude. The ridges are allowed to grow because of the nucleation at type-2 corners. The crystal front is therefore back to its original symmetry, but has increased in length in the direction that is allowed to grow at the re-entrant corners, as shown in the last crystal of Fig. 2(a). The ridges and the re-entrants could be both accelerated, but with different growth rates. The TPRE mechanism explains the six-fold ⟨112⟩ propagation and branching of ⟨112⟩ and ⟨110⟩ dendrites, but the model is not straightforward to predict the dendritic appearances. Wagner [4] proposed a more detailed growth mechanism (the W-model) of a faceted dendrite growth to explain the morphology. The growth of ridges is assumed to be limited. The type-1 re-entrant corners at the preferred growth directions disappear gradually at the beginning of the growth cycle, which results in the formation of three triangular corners with 60° after the corners have fully disappeared. Each part that is left behind now has formed a type-2 corner, and the type-2 corners start to grow. The growth continues in the described manner, as shown in Fig. 2(b). Repetition of the growth cycle gives the saw-tooth structure at the two sides of the faceted dendrite, which is widely observed in germanium and silicon melts. The W-model suggests that the dendritic tip keeps alternating with a flat surface or three 60° triangular corners, but the transition, i.e., the three 60° triangular corners such as the sequence 1 in Fig. 2(b), was not observed in the experiments.

Recently, experimental observations of twin related dendrites by *in situ* observation have been reported [15–21]; the dependence

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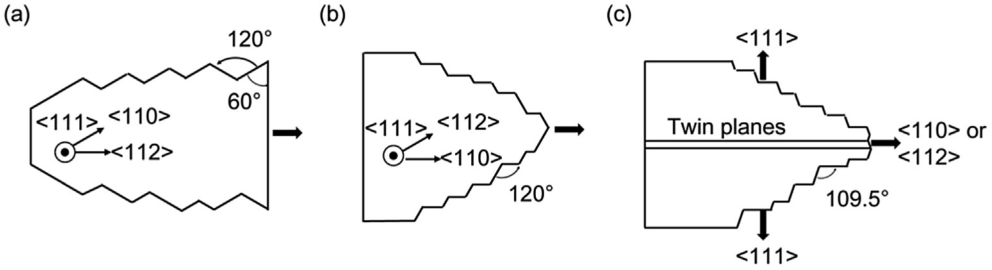

Fig. 1. Typical growth behaviors of faceted dendrites: (a) a ⟨112⟩ dendrite observed from ⟨111⟩ direction; (b) a ⟨110⟩ dendrite observed from ⟨111⟩ direction; (c) facet formation of a dendrite along the ⟨111⟩ directions.

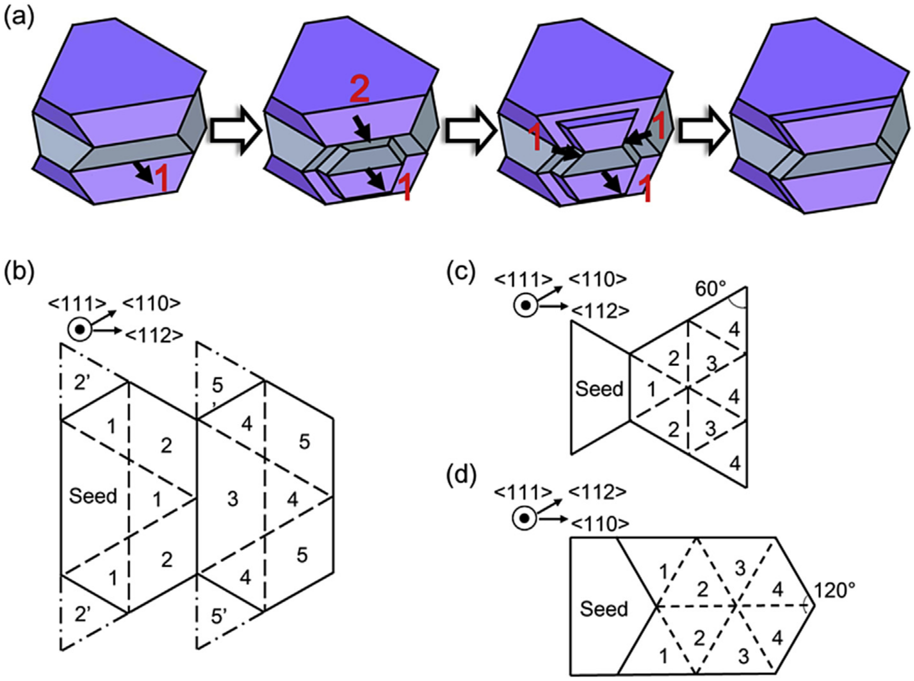

Fig. 2. Schematic of different growth models of a faceted dendrite: (a) the TPRE mechanism; (b) the W-model; (c) the F-model of a ⟨112⟩ dendrite; (d) the F-model of a ⟨110⟩ dendrite. The numbers in Fig. 2(a) indicate two types of re-entrant corners. The numbers in Fig. 2(b–d) indicate the growth sequence.

of growth direction on twin spacing and undercooling has also been studied [20]. Two modified growth models (the F-models) by Fujiwara et al. [18] have been proposed to explain different growth behaviors of ⟨112⟩ and ⟨110⟩ dendrites. The F-models are similar to the W-model that only the re-entrants are allowed to grow. In their model only the orientation of the dendrite is the preferred growth direction. For a ⟨112⟩ dendrite, as shown in Fig. 2(c), only one ⟨112⟩ is allowed to grow, so one 60°-triangular corner will form, as the sequence 1 in Fig. 2(c). Then the type-1 corners at the side of the tip start to propagate followed by the generation of a flat dendrite front with two 60°-horns, such as the sequence 2 in Fig. 2(c). Growth can continue with similar manners. Likewise, the F-model of the ⟨110⟩ dendrite is depicted in Fig. 2(d). With the same assumption, the crystal forms two 60°-triangular corners first, i.e., the sequence 1, and then is back to its original morphology but with the increasing length, as the sequence 2 in Fig. 2(d). The F-model for the ⟨112⟩ dendrite works well in Ref. [16]. Nevertheless, this implies that a platelet containing parallel twins might form triangular tips at any moment in the growth process, such as sequence 3 in Fig. 2(c), but such triangular tips were not reported in Ref. [16]. The F-model of the ⟨112⟩ dendrite suggests that the ⟨112⟩ dendrite becomes wider, but the width is almost constant in some experiments [8,18]. The F-model of the ⟨110⟩ dendrite seems to be more problematic. First, the model suggest that the dendrite tip alternates a 120°-tip or a 120°-reentrant corner during the growth process, but they were not found in the experiments. Second, the model fails for the growth process starting with a crystal with unequal facets. If a crystal with unequal facets grow in the manner as the F-model predicts, one should observe 60° corners on the appearance of a ⟨110⟩ dendrite. Third, the F-model fails to predict the side-branch morphologies.

To examine the correctness of the growth models, simulations of microstructure evolution could be of great help. The phase field model is widely applicable to model the dendritic growth process of weakly-anisotropic materials [22], and recently it has been successfully extended to model the solidification of highly anisotropic systems [23–26]. The anisotropic interfacial energy and kinetics are crucial for modeling facet formation of silicon growth. Eggleston et al. [25] used a regularized anisotropic function of interfacial energy for four-fold symmetry in two dimensions (2D). Later, Lin et al. [27] proposed a more simplified anisotropic function for facet formation of silicon with some success in 3D [26–28]. Meanwhile, several attempts have been conducted to simulate the dendritic growth of faceted materials [29–31], but the growth of faceted dendrites has