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Phase field method simulation of faceted dendrite growth with arbitrary symmetries

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Abstract: A numerical simulation based on a regularized phase field model is developed to describe faceted dendrite growth morphology. The effects of mesh grid, anisotropy, supersaturation and fold symmetry on dendrite growth morphology were investigated, respectively. These results indicate that the nucleus grows into a hexagonal symmetry faceted dendrite. When the mesh grid is above 640×640, the size has no much effect on the shape. With the increase in the anisotropy value, the tip velocities of faceted dendrite increase and reach a balance value, and then decrease gradually. With the increase in the supersaturation value, crystal evolves from circle to the developed faceted dendrite morphology. Based on the Wulff theory and faceted symmetry morphology diagram, the proposed model was proved to be effective, and it can be generalized to arbitrary crystal symmetries.
Key words: phase field method; strong anisotropy; faceted dendrite; Wulff theory; tip velocity; symmetry

1 Introduction

Interfacial energy anisotropy and mobility reflect the crystal structure of interfaces in materials. The crystallographic anisotropy has an important effect on the evolution dynamics and the final morphology structures in materials processing [1,2]. In particular, the anisotropy allows for the simulation of dendrite growth branches in solidification problems [3,4]. When anisotropy is weak for solid/liquid interfaces in most metallic materials, strong anisotropy often leads to facet interface structures such as in silicon, snowflakes or smooth surfaces. Faceted patterns appear in advanced and technological materials [5]. Faceted dendrites have attracted much attention due to their unique crystal structures particularly [6−9]. For example, on account of their aesthetics, snowflakes have attracted considerable interest for decades [10]. While robust theoretical interpretations of facet equilibrium shapes exist, the dynamical aspects of faceted pattern formation are still less understood. Thus, it is important to understand and investigate the mechanism by numerical simulation.

The most significant computational advantages of phase field method are that the explicit tracking of the interface is unnecessary, the interface curvature, anisotropy and kinetics parameters are implicitly incorporated in the phase field equation, and the phase field method has been proved to be a powerful tool for microstructure evolution simulation [11−16]. The method was developed by KARMA and RAPPEL [17] in 1996 for solidification of pure substances and later generalized by KARMA [18] for alloy solidification. However, in the early time, phase field method was mainly used to study the dendrite growth with weak anisotropy value [4,18]. When the anisotropy is so sufficiently strong missing orientations occur and sharp corners form in the Wulff shape [19−21]. This becomes ill-posed and reduces to un-regularized phase field equations. In order to recover accurately equilibrium shapes with corners due to missing orientations, in 2001, EGGLESTON et al [22] dealt with the ill-posedness

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through regularizing convexifying anisotropic surface energy, and simulated facet equilibrium shape with strong anisotropic interfacial energy. In an alternative phase-field approach, SUZUKI et al [23] simulated faceted crystal growth of silicon from the undercooled melt of silicon–nickel alloys. Recently, there also have been a number of attempts to regularize the phase-field equation [24−28]. For example, LIN et al [27] proposed a simplified anisotropic function, and then extended it to a 3D model.

In this work, based on Eggleston model [22], an effective regularized phase field model was presented to model faceted structure with six-fold symmetry, and the effects of mesh grid, anisotropy parameters, and supersaturation on faceted dendrite growth morphology were examined in detail. Furthermore, the fundamental idea of regularizing phase field model can be extended to generalize faceted dendrite morphology with arbitrary symmetries.

2 Phase field model

The equilibrium condition at solid/liquid interface is obtained by the Gibbs−Thomson equation [22]:

$$\frac{W(\theta)+W''(\theta)}{R(\theta)}=f^{\mathrm{L}}-f^{\mathrm{S}}=1-35\gamma\cos 6\theta \tag{1}$$

where $R(\theta)$ is the curvature radius of the solid/liquid interface, $W(\theta)(=W_0a(\theta))$ is the interface thickness to be anisotropic, $a(\theta)(=1+\gamma\cos(6\theta))$ is an anisotropic interface energy function, γ is the dimensionless anisotropy parameter, 6 is the folds of symmetry, f^{L} and f^{S} are the free energy densities of liquid and solid phases, respectively. When $\gamma\leq 1/35$, two sides of Eq. (1) are positive, and crystal morphology is smooth and continuity. When $\gamma>1/35$, the left side of Eq. (1) is negative as a result of the missing orientations, and discontinuous interface, which occurs concave similar to "ears". Besides, Eq. (1) can calculate the equilibrium shape [2,3] for two dimensions in parametric form as

$$x=W(\theta)\cos\theta-W'(\theta)\sin\theta \tag{2}$$

$$y=W(\theta)\sin\theta-W'(\theta)\cos\theta \tag{3}$$

Figure 1 shows the parametric plots for Wulff shape under different conditions. The unregularized Wulff shape is presented in dash red in Fig. 1(a). As shown for one typical strong anisotropy value, the equilibrium shape develops into sharp corners, and the high energy orientation for "ears" parts is missing. In order to simulate dendrite growth with strong anisotropy value, these "ears" must be removed, and the equation needs to be regularized. As seen in Fig. 1(b), missing orientations

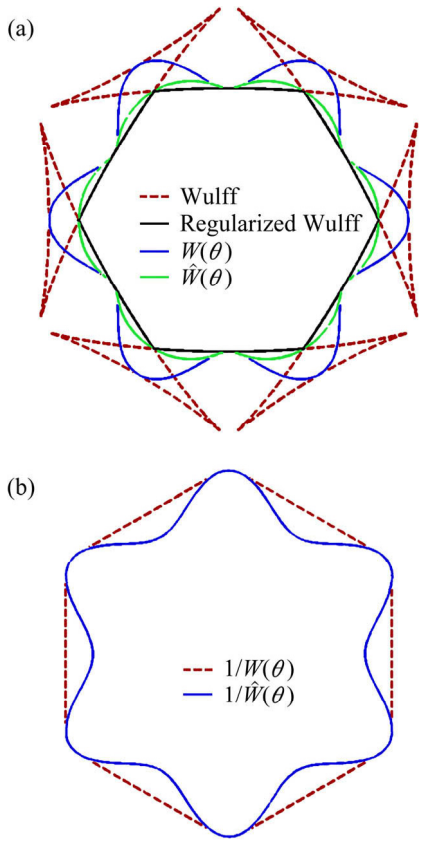

Fig. 1 Parametric plots: (a) Equilibrium shape of Wulff with "ears"(dash red line), equilibrium shape of regularized Wulff without "ears"(solid black line), plot of interface energy function $W(\theta)$ (solid blue line), plot of regularized interface energy function $\hat{W}(\theta)$ (solid green line); (b) Illustrating regularization method, inverse interface energy function ($1/W(\theta)$) and inverse regularization function $1/\hat{W}(\theta)$

in the equilibrium shape occur when the reciprocal $W(\theta)$ plot becomes concave. Therefore, in order to regularize the phase field equations, the interface energy within these missing orientations were regularized referring to method of EGGLESTON et al [22], as follows:

$$\hat{W}(\theta)=\begin{cases} W(\theta), & \frac{\pi}{3}i+\theta_{\mathrm{m}}\leq\theta\leq\frac{\pi}{3}(i+1)-\theta_{\mathrm{m}},\ i=0-5 \\ \dfrac{W(\theta_{\mathrm{m}})\cos\theta}{\cos\theta_{\mathrm{m}}}, & \frac{\pi}{3}i-\theta_{\mathrm{m}}<\theta<\frac{\pi}{3}i+\theta_{\mathrm{m}},\ i=0,3 \\ \dfrac{W(\theta_{\mathrm{m}})\cos(\theta-\pi/3)}{\cos\theta_{\mathrm{m}}}, & \frac{\pi}{3}i-\theta_{\mathrm{m}}<\theta<\frac{\pi}{3}i+\theta_{\mathrm{m}},\ i=1,4 \\ \dfrac{W(\theta_{\mathrm{m}})\cos(\theta-2\pi/3)}{\cos\theta_{\mathrm{m}}}, & \frac{\pi}{3}i-\theta_{\mathrm{m}}<\theta<\frac{\pi}{3}i+\theta_{\mathrm{m}},\ i=2,5 \end{cases} \tag{4}$$

As illustrated in Ref. [2], it replaces the anisotropy function in these regimes by choosing appropriately circular sections, which is shown in Fig. 1(b) for the case