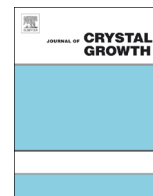




ELSEVIER

Contents lists available at ScienceDirect

## Journal of Crystal Growth

journal homepage: [www.elsevier.com/locate/jcrysgr](http://www.elsevier.com/locate/jcrysgr)

## Phase field modeling of facet formation during directional solidification of silicon film



H.K. Lin, H.Y. Chen, C.W. Lan\*

Department of Chemical Engineering, National Taiwan University, Taipei 10617, Taiwan

## ARTICLE INFO

Available online 28 February 2013

## Keywords:

A1. Facet  
 A1. Morphology  
 A1. Simulation  
 A1. Solidification

## ABSTRACT

Adaptive phase field modeling is conducted to study the facet formation during directional solidification of silicon film. The necessary condition for morphological instability is examined first based on the classic theory for the reported experiments. With a proper thermal gradient, the simulated onset velocity is found consistent with the experimental observations and the classic theory. The effects of anisotropy of kinetic coefficients and interfacial energy are also considered, and the simulated morphologies are significantly affected. The range of the kinetic cusp function affects the facet tips, while the anisotropy of interfacial free energy changes the wavelength of facets. Nevertheless, the simulation of kinetic undercooling on the facets is not successful, and the computational difficulty is discussed.

© 2013 Elsevier B.V. All rights reserved.

## 1. Introduction

The directional solidification of silicon has attracted a great attention in recent years due to its booming applications in photovoltaics. During solidification, the interface morphology plays a crucial role in defect formation and grain selection [1,2]. For silicon, the {111} planes tend to form facets during solidification, and the formation of facets and subgrain boundaries has particularly been focused [2]. Tokairin et al. [2,3] in situ observed the zigzag faceted morphology in a directional solidification system, and they found that the growth velocity and the wavelength of facets were influenced by the negative temperature gradient in the melt. They also observed that the stable spacing between the two facets increased with the growth velocity. Morphological transition from planar to zigzag facets and the critical growth velocities of (110), (112) and (100) planes in silicon were investigated by Fujiwara et al. [4] using a thin-film solidification system. Geis et al. [5] showed the faceted front with {111} planes in the zone-melting recrystallization of silicon. The density of subgrain boundaries, referred to as low-angle boundaries, could be controlled by the position of patterned optical absorbers. Pfeiffer et al. [6] reported the typical subgrain boundary networks and studied the mechanism of facet merging. They also derived a simple growth rate model to illustrate the dynamics of facet growth. Due to the more nucleation sites, the long facets enlarged and the short ones disappeared.

The phase field model (PFM) has become a powerful tool to describe the interface evolution during solidification in recent years [7]. However, for the simulation of silicon crystal growth, the anisotropy of the interfacial free energy and kinetics needs to be carefully considered. For the high anisotropy of the interfacial free energy, Eggleston et al. [8] derived a modified method for resolving missing orientations in the four-fold symmetry. Kasajima et al. [9] used this method to investigate the growth of a faceted silicon dendrite in an undercooled melt. Chen et al. [10] further used this function in their phase field model to study the grain competition of silicon; the facets in the <100> growth direction were simulated. Lin et al. [11] extended this method to three dimensions and discussed the effect of undercooling and the strength of anisotropy on the growth morphology of a dendrite.

On the other hand, the anisotropic kinetic effect in silicon could be more complicated. The big difference in the kinetic coefficient between the rough surface, e.g., (100), and the faceted surface (111) makes the simulation difficult, particularly as the high undercooling builds up on the facets. For the rough surface (100), the kinetic coefficient is about 0.12 m/(s K) [12]. However, for two-dimensional nucleation (2DN) growth on (111), the kinetic coefficient is three-order of magnitude smaller [13]. Furthermore, the kinetics is not linear as well. For the faceted growth, Uehara and Sekerka [14] assumed two functions, having sharp minima for special directions, to describe the anisotropic kinetic coefficient, and the result was in good agreement with the kinetic Wulff shapes. Weinstein and Brandon [15] also considered the 2DN mechanisms and introduced a cusp function to depict the kinetic coefficient. Miller et al. [16] further used a similar kinetic function to simulate the growth of Ge<sub>1-x</sub>Si<sub>x</sub> crystals. The behavior

\* Corresponding author. Tel./fax: +886 2 23633917.  
 E-mail address: cwlan@ntu.edu.tw (C.W. Lan).

of faceted growth was simulated and compared with experimental observations. However, the anisotropy of the interface energy was assumed to be small (0.03) in their simulation.

In this paper, we attempt to consider both anisotropies in the phase field model to simulate the faceted growth of silicon film observed in the reported experiments [3]. In addition to the necessary condition for the morphological instability, the effects of the anisotropies on the faceted morphology and the wavelength are discussed. The shortcomings of the present simulation are also addressed.

## 2. Growth conditions for morphological instability

For pure materials, the temperature gradient and the growth velocity are the two key parameters for morphological instability. However, as shown by Mullins and Sekerka [17,18], the negative mean thermal gradient  $G^*$  is the necessary condition for instability, where  $G^*$  is defined as

$$G^* = \frac{k_s G_s + k_l G_l}{k_s + k_l}, \quad (1)$$

where  $k_s$ ,  $G_s$ ,  $k_l$ , and  $G_l$  are the thermal conductivity and gradient of the solid and the liquid, respectively. From the stability criterion derived by Sekerka [19] and Chen et al. [20], we could estimate the critical wavelength ( $\lambda$ ) as a function of the mean thermal gradient ( $G^*$ ) and the anisotropic strength of the interfacial energy ( $\varepsilon_4$ ) as follows:

$$\lambda = 2\pi \sqrt{\frac{T_m d_0 (1 - 15\varepsilon_4)}{-G^*}}, \quad (2)$$

where  $T_m$  and  $d_0$  are the melting temperature and the capillary length, respectively, and  $\varepsilon_4$  is the strength of anisotropy for the interfacial free energy.

In the directional solidification experiments for silicon film, Tokairin et al. [3] also derived a one-dimensional temperature profile as a function of the growth velocity ( $V$ ) and the temperature gradient in the furnace ( $G$ ); the model was assumed pseudo-steady state and infinite sample length. They observed an onset velocity of 147  $\mu\text{m/s}$  for the faceted growth, and estimated the thermal gradient was about 8 K/mm. However, if we use this thermal gradient, we found that the weighted thermal gradient  $G^*$ , based on the thermal conductivities of the melt and solid, is always positive for the range of the velocity investigated in their experiments (50–250  $\mu\text{m/s}$ ). This implies that the interface should remain planar at  $G=8$  K/mm. In other words, their model did not give consistent thermal gradients in silicon to develop the facets.

In fact, the sample length in [3] was around 20 mm, and the silicon wafer was inside a quartz box for solidification. Because quartz has a much lower thermal conductivity than silicon, the thermal gradient inside silicon with both ends almost insulated could be much lower than that of the furnace ( $\sim 8$  K/mm), which was controlled by two graphite heaters. If two ends of the silicon wafer were assumed to be adiabatic, the thermal profile of the silicon wafer could be estimated from the heat exchange between the silicon and the ambient. Since the heat transfer from silicon to ambient is through quartz by conduction and then to the ambient by convective heat transfer of argon and thermal radiation, the effective heat transfer coefficient  $h_{\text{eff}}$  could be estimated as follows:

$$\frac{1}{h_{\text{eff}}} = \frac{1}{k_q/l_q} + \frac{1}{k_{\text{Ar}}/\delta_T + 4\sigma\varepsilon T_m^4}, \quad (3)$$

where  $k_q$  and  $k_{\text{Ar}}$  are the conductivities of quartz and argon, and  $l_q$  and  $\delta_T$  are the thicknesses of quartz and the thermal

**Table 1**  
Properties of silicon and environment.

Properties	Name	Value
$k_q$	Thermal conductivity of quartz (W/mK)	4.3
$k_{\text{Ar}}$	Thermal conductivity of argon (W/mK)	$1.7 \times 10^{-2}$
$l_q$	Thickness of quartz (m)	$10^{-3}$
$\delta_T$	Thermal boundary layer of argon (cm)	1 (Estimated)
$\sigma$	Stefan–Boltzmann constant (W/m <sup>2</sup> K <sup>4</sup> )	$9.6 \times 10^{-8}$
$\varepsilon$	Emissivity of silicon (dimensionless)	0.3

boundary layer of argon, respectively. Also,  $\sigma$  and  $\varepsilon$  are the Stefan–Boltzmann constant and the emissivity of quartz, respectively. The parameters in Eq. (3) are listed in Table 1. Based on these values,  $h_{\text{eff}}$  is about 80 W/m<sup>2</sup> K. Furthermore, if we assume the heat absorption from the hot zone is equal to the heat loss to the ambient, the average temperature gradient of silicon wafer for conduction is estimated to be only around 0.16G. This indicates that the actual temperature gradient in the silicon wafer is much smaller than that in the ambient.

On the other hand, if we still want to use the convenient analytical temperature distribution derived in [3], i.e., a pseudo-steady state approximation for a long sample, a simple way is to use a smaller ambient thermal gradient for simulation. As will be discussed shortly,  $G=1$  K/mm seems to be a proper value to use as we compare the calculated thermal gradients at the interface with those obtained by a transient simulation.

## 3. Phase field model

The phase field model used here is based on the thin-interface model proposed by Karma and Rappel [7]. The phase field variable  $\phi$  is set to 1 in the solid,  $-1$  in the melt, and 0 at the interface. To represent the model in dimensionless, the length is rescaled by  $W_0$ , which characterizes the interface thickness, and the time  $t$  is rescaled by  $\tau_0$ , which characterizes the atomic movement and the length. The velocity  $V$  is rescaled by  $W_0/\tau_0$ . The dimensionless variables are denoted by a superscript asterisk, unless otherwise stated. For the pulling velocity  $V_p$ , the dimensionless phase field equation could be written as follows:

$$\tau^*(\mathbf{n}) \left( \frac{\partial \phi}{\partial t^*} - V_p^* \frac{\partial \phi}{\partial x^*} \right) = \nabla^* \left[ W^*(\mathbf{n})^2 \nabla^* \phi \right] + \left[ \phi - \lambda_c u (1 - \phi^2) \right] (1 - \phi^2) + \partial_{x^*} \left[ |\nabla^* \phi|^2 W^*(\mathbf{n}) \frac{\partial W^*(\mathbf{n})}{\partial (\partial_{x^*} \phi)} \right] + \partial_{y^*} \left[ |\nabla^* \phi|^2 W^*(\mathbf{n}) \frac{\partial W^*(\mathbf{n})}{\partial (\partial_{y^*} \phi)} \right], \quad (4)$$

where  $\tau^*(\mathbf{n}) = \left[ a_s^2(\mathbf{n}) + \frac{\beta_0 D_m}{a_1 a_2 W_0} a_s(\mathbf{n}) a_k(\mathbf{n}) \right]$  for the thin-interface model, where  $\mathbf{n}$  is the normal direction at the interface and  $a_s(\mathbf{n})$  is the anisotropy function for the interfacial free energy,  $\beta_0$  is the kinetic coefficient,  $D_m$  is the mean diffusivity,  $a_1$  and  $a_2$  are constants [7], and  $a_k(\mathbf{n})$  is the anisotropy function for the kinetic coefficient. Moreover,  $V_p^*$  is the dimensionless pulling velocity and  $W^*(\mathbf{n}) = a_s(\mathbf{n})$ . Also,  $\lambda_c$  is a coupling constant between phase field and temperature field and  $u$  is the dimensionless temperature, i.e.,  $u = C_{p,l}(T - T_m)/\Delta H$ , where  $T$  is the temperature,  $C_{p,l}$  is the specific heat of the liquid, and  $\Delta H$  is the heat of fusion.

For small anisotropy ( $\varepsilon_4 < 1/15$ ), the interfacial anisotropy function for a four-fold system can be described as the following:

$$a_s(\mathbf{n}) = 1 + \varepsilon_4 \cos(4\theta), \quad (5)$$

where  $\theta$  is the angle between the local growth direction and the pulling direction. If the strength  $\varepsilon_4$  is greater 1/15, we convexify the polar plot of the reciprocal interfacial energy by a tangent line to resolve the missing orientation [8]. For the kinetic anisotropy function, we follow the relation proposed by Miller et al. [16], but

Download English Version:

<https://daneshyari.com/en/article/1790638>

Download Persian Version:

<https://daneshyari.com/article/1790638>

[Daneshyari.com](https://daneshyari.com)