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Micro structures in the grain evolution during solidification of silicon: Phase field calculations

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ABSTRACT

Two dimensional phase field simulations have been performed to study the influence of the growth kinetics and the surface energy on the growth behaviour of grains during solidification of Si. In particular, we studied the groove between two grains as recently observed by in situ observation [1]. Furthermore, we performed computations for different Σ boundaries and discuss the interplay between equilibrium of interfacial energies and growth kinetics.

1. Introduction

Despite the great importance of direct solidification of silicon and the large number of investigations there are still many open questions concerning the grain evolution.

Post-mortem analysis of the grain structure is one way for a better understanding of the growth kinetics. Most often these analyses are performed on wafers giving some statistics at a certain height but not the continuous evolution in time. Analysis in vertical direction has been performed e.g. by Prakash et al. [2] and more recently by Lin et al. [3]. However, only the situation after solidification and cooling can be analysed. A better path towards understanding the details is in-situ investigation which became recently available by improved synchrotron X-ray imaging to visualize the melt/solid interface of silicon [4]. Thus, it was possible to follow the creation and disappearance of facetted/facetted grooves [1].

For an understanding of the basic mechanisms a simulation on the microscopic length scale is required, which includes the effect of interface curvature. Here, phase field methods are the preferential ones. Chen et al. studied the grain competition in an undercooled melt with a simple anisotropy function for the solid/melt interfacial energy. Cantù et al. and Miller et al. studied a more advanced anisotropy function but simplified growth kinetics [5,6]. All aforentioned calculations have been two-dimensional approaches. Lin & Lan used a three-dimensional model, still with simplified anisotropy function and growth kinetics [7]. So far, all phase field calculations were based on the model of Warren et al. for computing the grain growth [8,9]. Also in this paper we use such a model and discuss in the end the limitations of this approach concerning the grain boundary orientation. Compared to our previous investigations [5,6] we update the solid/melt interfacial energy according to recent numerical and experimental results [10,11]. We also set the growth kinetics based on the results of molecular dynamics calculations [12]. The much more realistic input parameters enabled us to compare our calculations with the results of in situ investigations by Tandjaoui et al. [1].

2. Interfacial energies

In this paper we consider the (110) plane of silicon for 2D calculations (see Fig. 1). We need two kinds of interfacial energies for our computations: that of the melt/crystal interface and those of the grain/grain boundaries. In particular, we need the melt/crystal interface energy as a function of the orientation. Recently, the results of a molecular dynamics study [10] and of an experiment with in-situ observation [11] have been published. In both studies the equilibrium shape in the (110) plane was the result (see Fig. 2). The equilibrium shape represents the relative change of the interface

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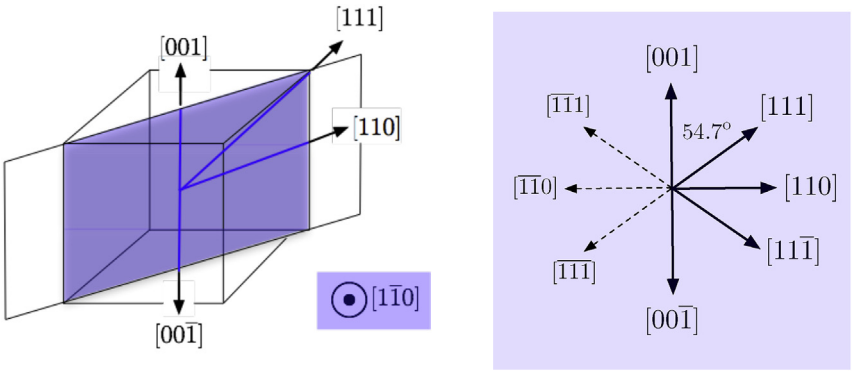

Fig. 1. Plane for calculations.

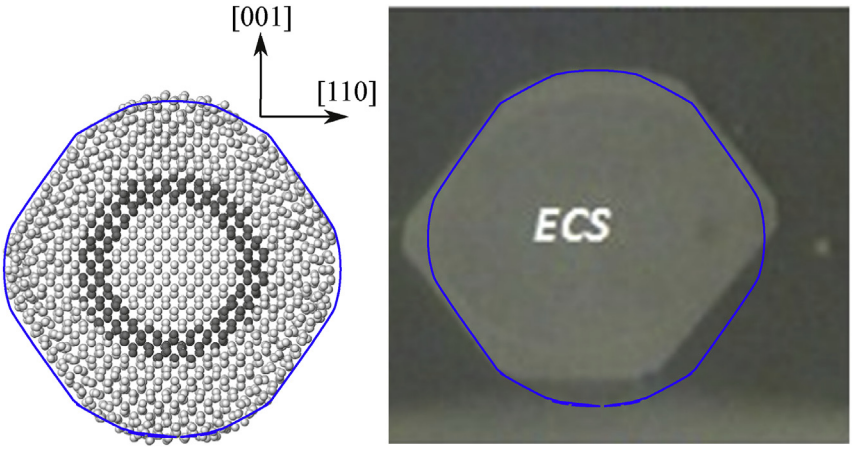

Fig. 2. Equilibrium shape for interface energy of Eq. (1) (blue line) in comparison with result of MD simulation (left [10]) and experiment (right [11]). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

energy with respect to orientation. Absolute value of interface energies were computed earlier for three orientations by means of molecular dynamics method [13]. Apte employed the cleaving wall method to extract the interfacial energies as follows: 0.42±0.02 J/m^2, 0.34±0.02 J/m^2, 0.35±0.03 J/m^2 for the {100}, {111}, and {110} planes, respectively. In the computations we need to represent the interface energy by a function, which is differentiable twice with respect to orientation. In order to recover an equilibrium shape close to the observed ones we made the following.

appoximation:

$$\gamma = 0.335\,\mathrm{J/m^2}\Big\{1. + 0.16(1 - \tanh(20(\vartheta - 50^\circ)) + 0.03(1 - \tanh(18(60^\circ - \vartheta)) - 0.02\sin^6(\vartheta - 1^\circ) - 0.05\cos^8(\vartheta) - 0.04\cos^{128}(\vartheta - 34^\circ)\Big\}. \quad (1)$$

The equilibrium shape given by this equation is shown in Fig. 2 as a blue line. Besides the equilibrium shape the three absolute values for the interface energy as given above were a criterium for setting up Eq. (1). We almost match the values given by molecular dynamics calculations as Eq. (1) yields 0.425 J/m^2 ({100}), 0.337 J/m^2 ({111}), and 0.348 J/m^2 ({110}).

The interface energy as a function of the orientation according to Eq. (1) is shown in Fig. 3. The curve is similar to the curve derived from bond density calculations [14]. We have four minima: two flat for {100} and {110} planes and two deep for {111} and {449} planes.

Grain boundary energies for silicon were computed by Kohyama and co-workers using a bond counting method [15]. More recently, molecular dynamics have been employed to obtain the energy at certain Σ boundaries [16]. In Fig. 4 we show the data points of the two kinds of calculations in the $(1\bar{1}1)$ plane. The original values of Kohyama et al. have been scaled by 0.65 to adapt them to the values of the molecular dynamics calculations. Thus, they are consistent with the absolute values of the melt/solid interfacial energy, which are also based on the results of molecular dynamics calculations. For small misorientations one can apply the Read-Shockley theory, where $\gamma_{GB} = \gamma^0_{GB}\frac{\Delta\theta}{\Delta\theta_m}\left(1 - \ln\left(\frac{\Delta\theta}{\Delta\theta_m}\right)\right)$, where $\Delta\theta$ and $\Delta\theta_m$ are the missorientation and the saturation, respectively. In Fig. 4 this energy is shown for $\gamma^0_{GB} = 0.68$ J/m^2 and $\Delta\theta_m = 28^o$ as a light grey curve. For the computations we use the values of the blue curve. This is discussed later in the context of the phase field model we use for computing the phase transition.

3. Growth kinetics

The growth velocity of a melt/solid interface is given by

$$v_n = \beta(\Delta T)\Delta T, \quad (2)$$

where ΔT is the undercooling at the considered point of the interface. The kinetic coefficient β depends on the growth