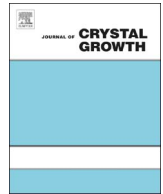




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# Three-dimensional analysis of dislocation multiplication during thermal process of grown silicon with different orientations

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## ABSTRACT

We used an advanced 3D model to study the effect of crystal orientation on the dislocation multiplication in single-crystal silicon under accurate control of the cooling history of temperature. The incorporation of the anisotropy effect of the crystal lattice into the model has been explained in detail, and an algorithm for accurate control of the temperature in the furnace has also been presented. This solver can dynamically track the history of dislocation generation for different orientations during thermal processing of single-crystal silicon. Four orientations, [001], [110], [111], and [112], have been examined, and the comparison of dislocation distributions has been provided.

## 1. Introduction

Dislocations in crystalline silicon have been identified as one of the most relevant defect centers for the efficiency of photovoltaic devices [1]. The demand for increased solar cell efficiencies necessitates a reduction in the number of dislocations. To reduce dislocations, the seeded growth of high-performance multicrystalline [2] or mono-like [3] silicon has been proposed. This technique can improve the quality of crystalline silicon, but the problem of the generation of dislocations has not yet been solved.

Many different attempts have been made to reduce dislocations, including the combination of differently orientated seeds [4], the replacement of multiple seeds with a single seed [5], the control of grain boundaries [6,7], the control of impurities [8], and so on. All of these can reduce the number of dislocations to some extent.

We are especially interested in the choice of the seed orientations in the method of combination of differently orientated seeds [4]. We aim to study the possibility of suppressing the generation of dislocations by changing only the crystal orientation, and to determine which orientation is the most beneficial for reducing dislocations. Furthermore, we are interested in the following: for the generation of dislocations, which orientation is not much affected by the later thermal processing after growth?

For the sake of convenience and simplification, we only considered several same-size cylindrical-shape ingots with different orientations in the axial direction. Certainly it is more reasonable to combine different-orientation crystals into one ingot, and study the dislocation generation

inside the different parts. However, the stress boundary conditions between the different parts will become complex due to the different crystal orientations. We will mainly use the simplified cases to illustrate the effect of the crystal orientations on the generation of dislocations, and the conclusions might be approximately applied to the multi-seed growth method. Furthermore, the simplified cases can easily help us study the sensitivity of dislocation generation on the crystal orientation during later thermal processing after growth.

Dislocation generation is a rather complex and totally nonlinear process. The simple critical resolved shear stress approach [9,10] cannot accurately describe the generation of dislocations. The Schmid factor method [11] under a uniform tangential stress field does not describe the dynamical generation process of dislocations. To accurately predict the effect of crystal orientation on the generation of dislocations, we used an advanced 3D dislocation model [12–14], which considers 12 slip directions, 144 cross slips, the immobilization of mobile dislocations, jog formation between different slip systems, and internal stress due to short-range interactions. This model can dynamically track the time evolution of the dislocation density with stress relaxation and strain hardening during the crystal growth process.

In this study, we use the 3D model to study the influence of crystal orientation on the generation of dislocations and try to clearly confirm which orientation is the most beneficial for the suppression of dislocation generation.

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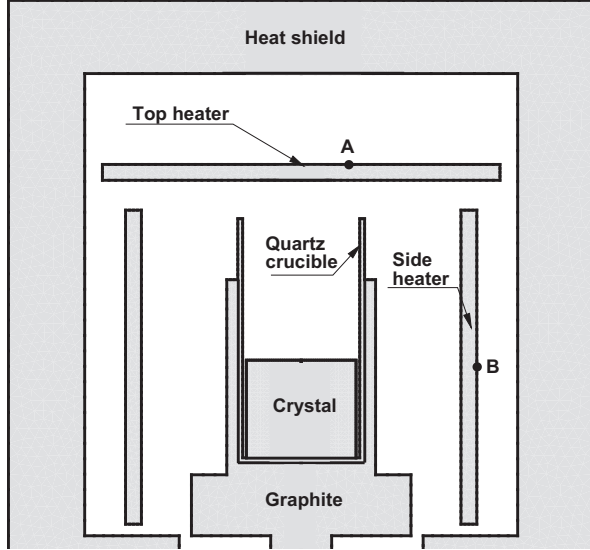
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**Table 1**  
Slip directions and slip planes for a cubic single crystal.

	1	2	3	4	5	6	7	8	9	10	11	12
$\sqrt{2}\mathbf{m}_i$	$[\bar{1}0\bar{1}]$	$[011]$	$[\bar{1}\bar{1}0]$	$[\bar{1}\bar{1}0]$	$[011]$	$[10\bar{1}]$	$[\bar{1}0\bar{1}]$	$[110]$	$[0\bar{1}1]$	$[10\bar{1}]$	$[0\bar{1}1]$	$[\bar{1}10]$
$\sqrt{3}\mathbf{n}_i$	$(\bar{1}\bar{1}1)$	$(\bar{1}\bar{1}1)$	$(\bar{1}\bar{1}1)$	$(\bar{1}\bar{1}1)$	$(\bar{1}\bar{1}1)$	$(\bar{1}\bar{1}1)$	$(\bar{1}\bar{1}1)$	$(\bar{1}\bar{1}1)$	$(\bar{1}\bar{1}1)$	$(111)$	$(111)$	$(111)$



**Fig. 1.** The configuration of the furnace [19]. The two monitoring points, A and B, are shown on the top and side heaters, respectively.

## 2. Formulations

The advanced 3D Alexander-Haasen model for dislocation multiplication can be referred to in papers [12–14]. This section will introduce only the incorporation of the anisotropic effect of the crystal lattice and the effect of crystal orientations into that model.

To incorporate the effect of the growth direction, the anisotropy effect of the crystal lattice has to be included. The elastically isotropic assumption characterized by the Young modulus and the Poisson ratio can no longer be used. For cubic single crystals with the Voigt notation used for stress and strain components, the anisotropic stress-strain relation can be given as follows in a Cartesian coordinate system  $x_1$ ,  $x_2$ , and  $x_3$ , which are coincident with the crystallographic axes,

$$\begin{Bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{Bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ & C_{11} & C_{12} & 0 & 0 & 0 \\ & & C_{11} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & C_{44} \end{bmatrix} \begin{Bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{Bmatrix}, \quad (1)$$

where  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$  are three independent elastic constants for cubic single crystals. The temperature dependencies of  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$  for single-crystal silicon can be found in the literature [15]. For convenience, we reproduce them here as follows:

$$C_{11} = 1.6564 \times 10^{12} \exp[-9.4 \times 10^{-5}(T - 298.15)], \quad (2-1)$$

$$C_{12} = 0.6394 \times 10^{12} \exp[-9.8 \times 10^{-5}(T - 298.15)], \quad (2-2)$$

$$C_{44} = 0.7951 \times 10^{12} \exp[-8.3 \times 10^{-5}(T - 298.15)], \quad (2-3)$$

where the unit of  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$  is Pa, and the unit of  $T$  is K.

In a practical crystal growth process, it is more convenient to use an arbitrary Cartesian coordinate system  $x'_1$ ,  $x'_2$ , and  $x'_3$ , in which  $x'_3$  is set to

be in the crystal orientation direction. In this arbitrary Cartesian coordinate system  $x'_1$ ,  $x'_2$ , and  $x'_3$ , the stress-strain relation can be given by

$$\begin{Bmatrix} \sigma'_1 \\ \sigma'_2 \\ \sigma'_3 \\ \sigma'_4 \\ \sigma'_5 \\ \sigma'_6 \end{Bmatrix} = \begin{bmatrix} C'_{11} & C'_{12} & C'_{13} & C'_{14} & C'_{15} & C'_{16} \\ & C'_{22} & C'_{23} & C'_{24} & C'_{25} & C'_{26} \\ & & C'_{33} & C'_{34} & C'_{35} & C'_{36} \\ & & & C'_{44} & C'_{45} & C'_{46} \\ & & & & C'_{55} & C'_{56} \\ & & & & & C'_{66} \end{bmatrix} \begin{Bmatrix} \varepsilon'_1 \\ \varepsilon'_2 \\ \varepsilon'_3 \\ \varepsilon'_4 \\ \varepsilon'_5 \\ \varepsilon'_6 \end{Bmatrix}, \quad (3)$$

where the components of the elastic matrix  $C'_{ij}$  are related to the three independent elastic constants  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$ , and the direction cosines of  $x'_i$  vs.  $x_j$  between the above two coordinate systems. The formulations of  $C'_{ij}$  has been provided by Miyazaki [16].

In many practical crystal growth processes, axisymmetrically shaped crystals are grown. To conveniently describe the crystal shape, a cylindrical coordinate system  $x_1^*(=r)$ ,  $x_2^*(=\theta)$ ,  $x_3^*(=z)$  is generally adopted and the coordinate  $x_3^*$  is also normally set to be in the crystal orientation direction, i.e.,  $x_3^*(=z) = x'_3$ . The stress-strain relationship in the cylindrical coordinate system can be expressed as

$$\begin{Bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{zz} \\ \sigma_{\theta z} \\ \sigma_{zr} \\ \sigma_{r\theta} \end{Bmatrix} = \begin{bmatrix} C^*_{11} & C^*_{12} & C^*_{13} & C^*_{14} & C^*_{15} & C^*_{16} \\ & C^*_{22} & C^*_{23} & C^*_{24} & C^*_{25} & C^*_{26} \\ & & C^*_{33} & C^*_{34} & C^*_{35} & C^*_{36} \\ & & & C^*_{44} & C^*_{45} & C^*_{46} \\ & & & & C^*_{55} & C^*_{56} \\ & & & & & C^*_{66} \end{bmatrix} \begin{Bmatrix} \varepsilon_{rr} \\ \varepsilon_{\theta\theta} \\ \varepsilon_{zz} \\ \varepsilon_{\theta z} \\ \varepsilon_{zr} \\ \varepsilon_{r\theta} \end{Bmatrix}, \quad (4)$$

where the components of the elastic matrix  $C^*_{ij}$  are determined from  $C'_{ij}$ , the covariant metric tensor  $g_{\alpha\beta}$ , and the derivatives  $\partial x_i^*/\partial x'_j$ . The formulation of  $C^*_{ij}$  has been provided by Miyazaki [16].

The anisotropic stress calculation has to be solved in a three-dimensional system and requires a lot of computational time. As pointed out in a previous study [17], two simplifications can be adopted to reduce the total computational time, introducing just a small error of less than 6%. The first simplification is that the shear stresses  $\sigma_{\theta z}$  and  $\sigma_{r\theta}$  are considerably smaller than all of the other stress components and can therefore be neglected [17,18]. The second simplification is that all of the terms involving a trigonometric function of  $n\theta$  can be neglected after the drop power transformation of the trigonometric functions, which is equivalent to performing an average over  $2\pi$ . Therefore, a simplified 2D stress-strain relation including the anisotropy effect of the elastic constants can be written as follows:

$$\begin{Bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{zz} \\ \sigma_{rz} \end{Bmatrix} = \begin{bmatrix} C_{11} + \lambda_{11} & C_{12} + \lambda_{12} & C_{12} + \lambda_{13} & \lambda_{14} \\ & C_{11} + \lambda_{22} & C_{12} + \lambda_{23} & \lambda_{24} \\ & & \text{Symm.} & C_{11} + \lambda_{33} \\ & & & C_{44} + \lambda_{44} \end{bmatrix} \begin{Bmatrix} \varepsilon_{rr} \\ \varepsilon_{\theta\theta} \\ \varepsilon_{zz} \\ \varepsilon_{rz} \end{Bmatrix}, \quad (5)$$

where  $\lambda_{ij}$  denotes the anisotropy effect in a silicon single crystal, which is different for different orientations. For example, Miyazaki [16] has provided the following expression:

$$C^*_{11} = C'_{11} \cos^4 \theta + C'_{22} \sin^4 \theta + 2(C'_{12} + 2C'_{66}) \cos^2 \theta \sin^2 \theta + 2(C'_{16} \cos^2 \theta + C'_{26} \sin^2 \theta) \sin 2\theta, \quad (6)$$

where  $C'_{ij}$  is the constant matrix of Eq. (3) for an arbitrary Cartesian coordinate system  $x'_1$ ,  $x'_2$ , and  $x'_3$ . The drop power transformation of the trigonometric functions can be performed as follows:

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