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Numerical analysis of the relation between dislocation density and residual strain in silicon ingots used in solar cells

S. Nakano[a,*], B. Gao[a], K. Jiptner[b], H. Harada[b], Y. Miyamura[b], T. Sekiguchi[b], M. Fukuzawa[c], K. Kakimoto[a]

[a] Research Institute for Applied Mechanics, Kyushu University, 6-1 Kasuga-koen, Kasuga, Fukuoka 816-8580, Japan
[b] National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan
[c] Kyoto Institute of Technology, Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan

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ABSTRACT

We have developed a three dimensional Haasen-Alexander-Sumino model to investigate the distribution of dislocation density and residual strain in Si crystals and compared the calculation results with experimental data performed in mono-like and multicrystalline silicon ingots. The results show that the residual strain in a multicrystal is lower than in a mono-like crystal, whereas the dislocation density in the multicrystal is higher than that in the mono-like crystal. This phenomenon is due to the relation between dislocation density and residual strain caused by the difference of activated slip systems in a mono-like crystal and a multicrystal.

1. Introduction

The use of solar energy is increasing and is critical to our efforts to address global warming owing to the use of fossil fuels. The widespread use of photovoltaic systems has made it necessary to reduce manufacturing costs and improve conversion efficiency. The directional solidification method is the most widely used method for growing multicrystalline silicon (mc-Si) ingots for photovoltaic materials. The main advantages of this method are its low cost and high throughput. To fulfill the recent requirement not only to reduce the cost but also to increase the conversion efficiency, attractive crystal growth methods, such as high-performance mc-Si method [1] and the seeded directional solidification (seed-cast) method [2,3] have been proposed. The seed-cast method has attracted much attention over the years. Seed crystals are placed at the bottom of a crucible and mono-like Si ingots are grown using the directional solidification method. However, this method necessarily provokes small angle grain boundaries between the seed crystals [4,5]. These small angle grain boundaries may cause the generation of dislocations. Miyamura et al. have proposed the single seed-cast technique and have developed this method [6,7]. Presently, the conversion efficiency of mono-like Si which was grown by single seed-cast method is close to that of monocrystalline materials, such as Czochralski silicon crystals [8,9].

For mc-Si or mono-like Si, which is grown by the directional solidification method, the dislocation density is known to decrease the conversion efficiency [10,11], whereas the residual stress can cause the crystals to fracture [12,13]. To increase the conversion efficiency and yield rate of solar cells, it is necessary to reduce the dislocation density and residual stress in the Si crystals.

Evaluating the quality of crystals is important in experiments [14–17]; however, it is not easy to estimate the dislocation generation and behavior of residual stress during the growth process. Analyzing numerical simulations can help us understand this important problem. Therefore, via numerical simulation, we can improve the furnace design and optimize the growth conditions, thereby improving the quality of Si crystals.

In this paper, we aim to clarify the relation between dislocation density and residual strain in mono-like Si and mc-Si using experimental verification.

2. Evaluation process

2.1. Experimental condition

Fig. 1 shows the schematic of the directional solidification furnace. The directional solidification furnace comprised a silicon melt, a crystal, crucibles, pedestals, heat shields, and heaters. The two measuring points for temperature are located on the top and side heaters, respectively. We grew two mono-like crystals (Crystal 1 and Crystal 2) by directional solidification using (001)-oriented single seed crystal [15,16]. In this method, the heaters are moved upward to grow the crystal, while the heater power is held constant until the solidifica-

* Corresponding author.
E-mail address: snaka@riam.kyushu-u.ac.jp (S. Nakano).

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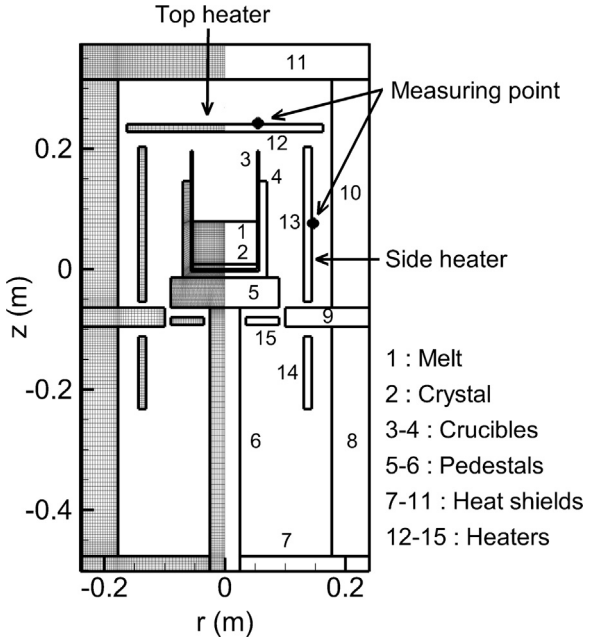

Fig. 1. Schematic of the directional solidification furnace.

tion process is complete, at which point it is decreased. The crystal was 75 mm high with a diameter of 105 mm.

Fig. 2 shows the growth recipe of the heater temperature and crucible positions in the experiment [16]: temperature profile at measuring points of top and side heater and crucible position at the bottom as a function of time. We require that temperatures at two measuring points have the same histories as shown in Fig. 2. We maintained the same melting and solidification conditions for both crystals and only changed the cooling rate below 900 °C. The cooling rate for Crystal 1 was about 12 °C/min, whereas for Crystal 2 it was about 5 °C/min below 900 °C.

Two 1.5-mm-thick ingots were cut from the (110) surface to measure the residual strain in the ingot. The residual strain was measured using a scanning infrared polariscope (SIRP). The step size is 200μm. The residual strain was evaluated as the absolute difference of refractive indices $|\Delta n|$ by SIRP. The larger the residual strain is, the larger is $|\Delta n|$. Details of the SIRP measurements have already been reported elsewhere [18,19].

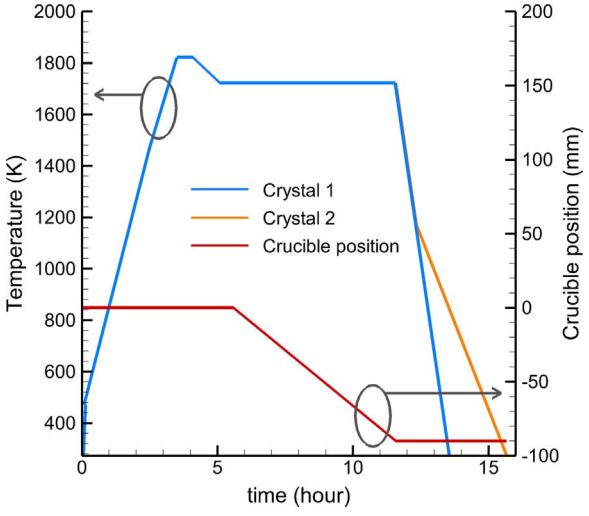

Fig. 2. Growth recipe of the heater temperature and crucible positions in the experiments. Temperature profile at measuring points of top and side heaters and crucible position at the bottom as a function of time.

Dislocation density was determined by optical microscopy after Secco etching for 90 s [20].

2.2. Model description and computation method

A transient global model was developed to describe the directional solidification process and to study the global heat transfer in the entire furnace as a function of time, including the convective heat transfer in the silicon melt, the conductive heat transfer in all the solid components, and the radiative heat transfer between all diffusive surfaces of the furnace. The geometry of the furnace configuration is axisymmetric. A dynamic interface tracking method was also used to obtain the shape of the solid–liquid interface. Details of the calculations have already been reported elsewhere [21–23]. Fig. 3(a) shows the evolution of heater power and the crucible position at the bottom, and Fig. 3(b) shows the temperature profile at a measuring point of the top heater with respect to time in the calculations. The cooling rate for Crystal 1 was about 6.1 °C/min, whereas for Crystal 2 it was about 2.2 °C/min below 900 °C. The cooling rate in the experiments and calculations differ; however, we can qualitatively compare the effect of cooling rate below 900 °C.

We have developed a three-dimensional (3D) Haasen-Alexander-Sumino (HAS) isotropic model [24–28] to analyze the behavior of dislocations and residual strain for mono-like Si or mc-Si crystal during the growth process. A brief explanation of the equations is given below. Details on the calculations are given elsewhere [24–28].

A silicon crystal has twelve slip directions because of its fcc structure [28,29]. The resolved shear stress $\tau^{(\alpha)}$ in the α slip direction can be obtained using the tensor transformation technique [29]. The creep strain rate $d\varepsilon_{pl}^{(\alpha)}/dt$ is obtained by Orowan's relation [30]:

$$\frac{d\varepsilon_{pl}^{(\alpha)}}{dt} = N_m^{(\alpha)} v^{(\alpha)} b, \tag{1}$$

where $N_m^{(\alpha)}$ is the mobile dislocation density, i.e. the number of mobile dislocations per unit area associated with the α slip direction, b is Burger's vector, and $v^{(\alpha)}$ is the slip velocity of these dislocations.

The rate of the mobile dislocation density in the α slip direction is

$$\frac{dN_m^{(\alpha)}}{dt} = K N_m^{(\alpha)} v^{(\alpha)} \tau_{eff}^{(\alpha)} + K^* N_m^{(\alpha)} v^{(\alpha)} \tau_{eff}^{(\alpha)} \sum_{\beta \neq \alpha} f_{\alpha\beta} N_m^{(\beta)} - 2 r_c N_m^{(\alpha)} N_m^{(\alpha)} v^{(\alpha)}, \tag{2}$$

where $\tau_{eff}^{(\alpha)}$ is the effective stress for dislocation multiplication in α slip direction, K and K^* are multiplication constants [26–28], and r_c is the effective dipole half width [26–28]. The $f_{\alpha\beta}$ coefficients are either one or zero. On the right-hand side of Eq. (2), the first term denotes the dislocation increase caused by the glide on the slip plane, the second term denotes the formation of jogs on a screw dislocation and the consequent expansion through spiral formation, and the third term denotes dislocation immobilization.

The slip velocity of the dislocation $v^{(\alpha)}$ is

$$v^{(\alpha)} = v_0 \left(\frac{\tau_{eff}^{(\alpha)}}{\tau_0}\right)^m \exp\left(-\frac{U}{k_b T}\right), \tag{3}$$

where the velocity prefactor $v_0 = 5000 m/s$, $\tau_0 = 1 MPa$, $m = 1$, the activation energy for dislocation motion $U = 2.2 eV$, and Boltzmann's constant $k_b = 8.617 \times 10^{-5} eVK^{-1}$[31]. The effective stress is

$$\tau_{eff}^{(\alpha)} = \langle \tau^{(\alpha)} - \tau_i^{(\alpha)} - \tau_b^{(\alpha)} \rangle, \tag{4}$$

where $\tau^{(\alpha)}$ is the resolved shear stress, $\tau_i^{(\alpha)}$ is the necessary stress for overcoming short-range obstacles, and $\tau_b^{(\alpha)}$ is the internal long-range elastic stress, which is caused by mobile dislocations [26–28,31]. If $x > 0$, $\langle x \rangle = x$, and if $x \leq 0$, $\langle x \rangle = 0$.

The short- and long-range interactions are given as follows [31]:

$$\tau_i^{(\alpha)} = \mu b \sqrt{\sum_\beta a_{\alpha\beta} (N_m^{(\beta)} + N_i^{(\beta)})}, \tag{5}$$