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Three-dimensional analysis of dislocation multiplication in single-crystal silicon under accurate control of cooling history of temperature

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ABSTRACT

Dislocation multiplication in single-crystal silicon during heating and cooling processes was studied by three-dimensional simulation under accurate control of the temperature history. Three different cooling temperature histories were designed. The results showed that the cooling rate in the high-temperature region has a large effect on the final dislocations and residual stress. The most effective method to reduce dislocations is to use a slow cooling rate in the high-temperature region.

1. Introduction

The photovoltaic industry is in a phase of rapid growth, and has increased by over 30% per year over recent years [1]. Two of the main challenges of today's photovoltaic industry are cost reduction and the increase of solar cell efficiencies. Solar cell efficiencies can be affected by many factors, such as impurities, point defects, grain boundaries, and dislocations [2]. Dislocations have been identified as one of the most efficiency-relevant defect centers in crystalline silicon for photovoltaic devices [3]. The requirement for an increase of solar cell efficiencies necessitates a reduction of dislocations.

In crystalline silicon, dislocations usually take place in the high-temperature processes of crystal growth, such as crystallization and cooling processes. The crystallization process usually contributes slightly to the increase of dislocations, whereas the cooling process has a large effect on the increase of dislocations [4]. Hence, many studies have concentrated on the cooling process [5–8]. However, the results are not consistent. Slow cooling was suggested for obtaining low dislocation density in GaP/Si heterostructures [5] and in SiGe layers grown by liquid phase epitaxy [6]. Fast cooling was suggested for obtaining low dislocation density in Pb [7] and Si crystal growth [8] from the melt. This discrepancy shows that the effect of the cooling process on the multiplication of dislocation is complex and different for different materials, growth furnaces, and growth processes. To better understand the relationship between the cooling rate and dislocation, it is essential to study the effect of the cooling process on the increase of dislocations from the perspective of accurate control of temperature history inside furnace according to a pre-designed curve.

Since the temperature history inside furnace has been predesigned, the electric current, i.e., heater power, has to be automatically adjusted. This can be realized by an automatic control technique, such as proportional–integral–differential (PID) control. A numerical solver, which simulates that automatic control process, has been developed for accurately control of temperature history inside furnace. We monitored two points on two heaters, and required that the temperatures at the two monitored points evolve according to a pre-designed temperature history.

In this paper, we used this solver to study the effect of cooling process on dislocation multiplication, and attempt to clarify the following problem: what is the most effective method to reduce dislocations when the cooling process is designed?

2. Numerical simulation

2.1. Furnace configuration

An axisymmetric unidirectional solidification furnace was used. An axisymmetric single-crystal silicon ingot was placed in a quartz

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0022-0248/

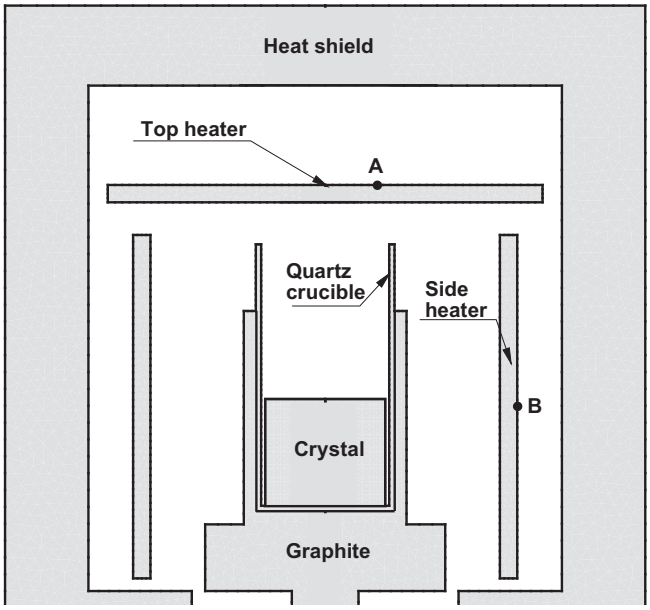

Fig. 1. Configuration of furnace. The two monitoring points A and B are shown on the top and side heaters, respectively.

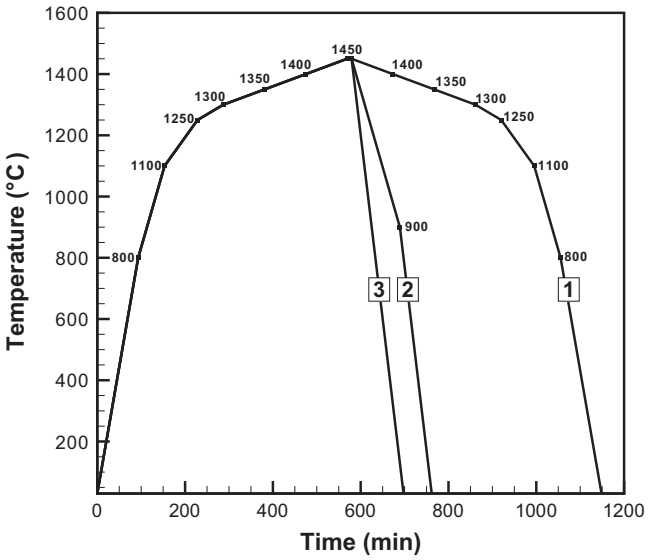

Fig. 2. Designed temperature history at monitoring points.

crucible. To accurately track dislocations without ambiguity in imposing boundary conditions between the quartz crucible and crystal, a small gap of 3 mm was maintained between the crucible and crystal. The inner diameter of the crucible was 96 mm. The ingot was dislocation free at room temperature. The basic configuration of the furnace is shown in Fig. 1. The two monitoring points A and B are shown on top and side heaters, respectively.

2.2. Design of temperature history

To determine the influence of the cooling process on dislocation multiplication, three different cooling processes were designed, as shown in Fig. 2. The cooling rates of cases 1, 2, and 3 were different at the initial stage of the cooling process, but were the same at the final stage of the cooling process. The heating process was the same for all three cases.

To homogenize the temperature distribution inside the furnace, we required that the temperature histories at monitoring points A and B were the same. It is a nonlinear optimization problem defined by two sets of parameters: the input parameters of top heater power Q_{top} and bottom heater power Q_{bottom}, and the output parameters of the temperatures at points A (T_A) and B (T_B). The optimization target at any time t is $T_A(Q_1, Q_2, t) = T_B(Q_1, Q_2, t) = T_{design}(t)$.

2.3. Temperature field calculation

Calculation of the temperature field inside the furnace involves conductive heat transfer in all solid components and radiation heat transfer in all enclosures of the furnace. The radiative heat exchange in all radiative enclosures was modeled based on the assumption of diffuse-gray surface radiation. Convective cooling by argon gas was ignored in the calculation of the thermal fields. For details of the global heat transfer, refer to Liu and Kakimoto [9].

2.4. Obtained temperature and heater power histories

The nonlinear optimization for the cooling process of case 3 outputs two monitoring-point temperatures (T_A and T_B) and the two heater powers (Q_{top} and Q_{bottom}), which are shown in Fig. 3. The calculated temperatures fitted the designed temperature well except in the low-temperature region of the cooling process ($<600\,^{\circ}C$). The main reason for the difference between the designed and calculated temperatures in the low-temperature region of the cooling process is that the temperature cannot linearly decrease in the low-temperature region, as in the designed system, because the heat capacity of the furnace already decreases so much. The top power is much higher than the bottom power.

2.5. Three-dimensional simulation of dislocations in silicon

Thermal stress and dislocation multiplication have been studied by numerical simulations in various crystal growth processes [10–23]. However, most of the simulations for the multiplication of the dislocation assumed uniaxial creep or single slip, and ignored many factors, such as the immobilization of mobile dislocations, the jog formation between different slip systems and its influence on dislocation generation, or the internal stress owing to short-range interactions from the total dislocation density. In our previous papers [4,24,25], we included all of the above factors and studied the activated mechanics of slip systems in different growth directions under different cooling fluxes. The detailed formulas and parameters for the three-dimensional simulation of dislocations in silicon can be found in those papers [4,24,25]. A brief introduction was given as follows:

Silicon crystals have 12 slip directions. The resolved shear stress along the α slip direction can be obtained by

$$\tau^{(\alpha)} = \mathbf{s}^{(\alpha)} \times \boldsymbol{\sigma}_{\text{cart}} \times \mathbf{n}^{(\alpha)}, \tag{1}$$

where $\tau^{(\alpha)}$ is the resolved shear stress, $\boldsymbol{\sigma}_{\text{cart}}$ is the stress tensor in Cartesian coordinate system, $\mathbf{s}$ is the unit vector of the slip direction in the Cartesian coordinate system, and $\mathbf{n}$ is the unit normal vector of the slip plane in the Cartesian coordinate system.

After the resolved shear stress $\tau^{(\alpha)}$ is obtained, the creep strain rate $d\varepsilon_{pl}^{(\alpha)}/dt$ is given by the Orowan relationship [26]

$$d\varepsilon_{pl}^{(\alpha)}/dt = N_m^{(\alpha)} \boldsymbol{\nu}^{(\alpha)} b, \tag{2}$$

where the subscript m denotes the mobile dislocation, the superscript α denotes the slip direction, b is the Burger's vector, N is the