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Quality evaluation of multi-crystalline silicon ingots produced in a directional solidification furnace with different theories

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ABSTRACT

Three methods for evaluating the quality of silicon ingots produced in a directional solidification furnace were compared. The methods are based on the thermo-elastic theory, thermo-plastic theory and thermo-creep theory. The methods use the von Mises stress, the accumulated viscoplastic strain, and the dislocation density as the evaluation parameters of ingot quality, respectively. The evaluation parameters and their distributions were calculated in the growing silicon ingots during the solidification process and in the grown ingots during the annealing process. The distributions of the quality evaluation parameters in the growing ingots are similar in the solidification process for the three methods. The evaluation method based on thermo-elastic theory is recommended because of its higher computational efficiency than the other two methods. However, in the ingot annealing process the distributions of the evaluation parameters vary considerably with the three methods. The thermo-plastic theory and the thermo-creep theory are more suitable for the whole process. It demonstrates that large dislocation density is generated in the ingot during the annealing process.

1. Introduction

The solar photovoltaic (PV) market is rapidly developing. At present, multicrystalline silicon ingots produced by the directional solidification (DS) method are the most widely used semiconductor substrate for manufacturing solar cells because of its cost-effectiveness. Defects such as impurities and dislocations in the multicrystalline silicon ingots decrease the lifetime of minority carriers [1], resulting in the reduction of the conversion efficiency of solar cells. The generation of dislocations in the ingot during the crystal growth process mainly depends on the distribution and magnitude of thermal stress in the ingot. To optimize the directional solidification process and the thermal field in the solidification furnace, a reliable method to evaluate and analyze the ingot quality during crystal growth is required. However, the mechanical behavior of the silicon ingot at high temperature is very complex and experimental methods to measure the mechanical properties are limited. Thus, different evaluation methods are used to predict the ingot quality during the solidification and annealing process at high temperature. The thermo-elastic method is a widely used method to evaluate the ingot quality [2–4], in which the von Mises stress is used as an evaluation parameter. M'Hamdi et al. [5–7] studied multi-crystalline silicon quality by using the thermo-plastic method, and used the accumulated viscoplastic strain to evaluate the crystal quality. The dislocation density was used to evaluate the crystal quality by Miyazaki et al. [8–11] and Chen et al. [12,13] with the thermo-creep method. Because different theories are used in these methods, the conclusions drawn from these methods are also different. However, to our knowledge, there has been no study comparing these methods, and the similarities and differences among them have not been clarified. Therefore, it is necessary to compare and analyze the different ingot quality evaluation methods.

2. Description of the evaluation methods

2.1. Numerical model of heat transfer

We calculated the thermal field in a silicon ingot growing in an industrial DS furnace. The whole transient process including the solidification process and the annealing process is taken into account. The time scale we used in our simulation is the same as that of the real process. For the purpose of saving the computational resources, the square crucible is equivalently simplified to a cylindrical shape, and the thermal resistance is kept unchanged in the DS system. This simplification is widely used in literatures [14–16] and has been validated by experiment [17]. The configurations and computational

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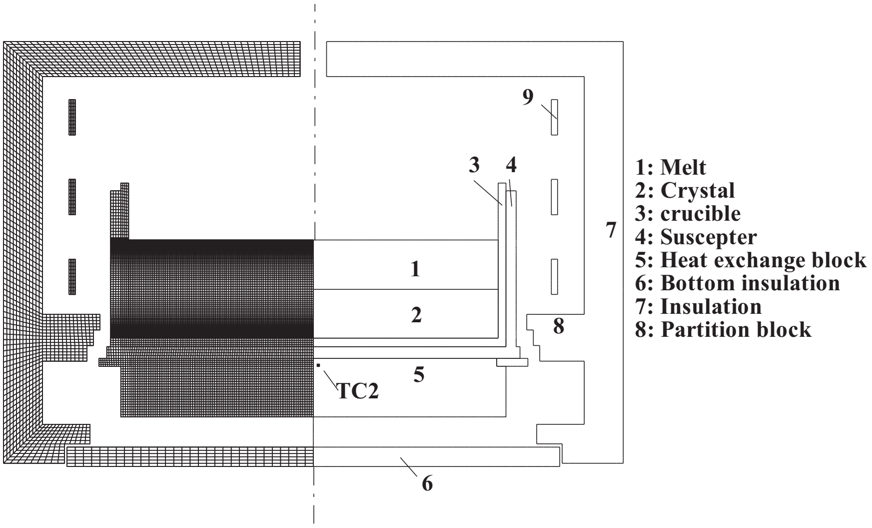

Fig. 1. Configurations and computational grids of the hot zone in an industrial-scale DS furnace.

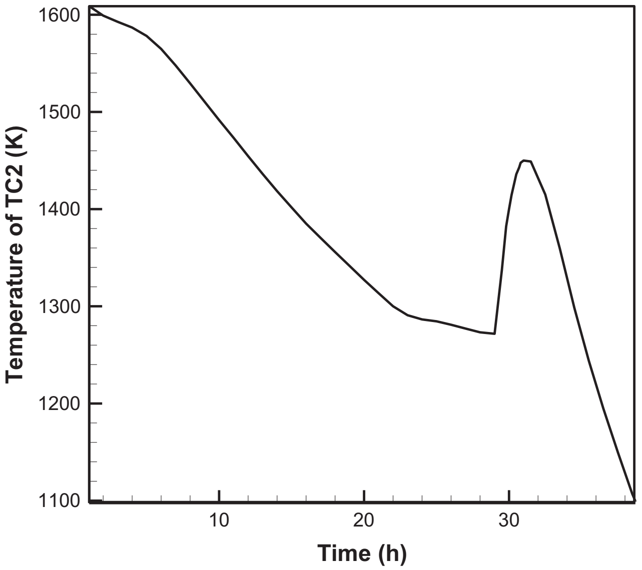

Fig. 2. Evolution of temperature at the crucible bottom (TC2).

grids of the hot zone in the furnace are shown in Fig. 1. The governing equations and algorithms for the global modeling of heat transfer in the furnace have been published elsewhere [18,19]. A thermocouple is installed at the upper center of the heat exchange block to monitor the temperature at the crucible bottom (TC2), which is shown in Fig. 1. The numerically obtained evolution of TC2 is shown in Fig. 2, which is very close to the experiment data [17]. The solidification rate is calculated in our simulation and we obtained it with an average value of about 1.0 cm per hour.

2.2. Numerical model of ingot quality evaluation

In the silicon ingot region, by applying the axisymmetric displacement-based model presented by Fainberg and Leister [20], the governing equations for the momentum balance in an axisymmetric case can be written as [2]

$$\frac{1}{r}\frac{\partial}{\partial r}(r\sigma_{rr})+\frac{\partial}{\partial z}(\sigma_{rz})-\frac{\sigma_{\varphi\varphi}}{r}=0, \tag{1}$$

$$\frac{1}{r}\frac{\partial}{\partial r}(r\sigma_{rz})+\frac{\partial}{\partial z}(\sigma_{zz})=0, \tag{2}$$

where σ_{rr}, σ_{zz}, $\sigma_{\varphi\varphi}$ are the normal stresses in the radial, axial, and azimuthal directions, respectively, and σ_{rz} is the shear stress.

We used Hooke's law for the elastic strain, and the stress–strain relationship is given by

$$\begin{pmatrix}\sigma_{rr}\\ \sigma_{\varphi\varphi}\\ \sigma_{zz}\\ \sigma_{rz}\end{pmatrix}=\begin{pmatrix}c_{11} & c_{12} & c_{13} & 0\\ c_{12} & c_{22} & c_{23} & 0\\ c_{13} & c_{23} & c_{33} & 0\\ 0 & 0 & 0 & c_{44}\end{pmatrix}\begin{pmatrix}\varepsilon^e_{rr}\\ \varepsilon^e_{\varphi\varphi}\\ \varepsilon^e_{zz}\\ \varepsilon^e_{rz}\end{pmatrix}, \tag{3}$$

where c_{ij} are the elastic coefficients of the silicon ingot. The values of c_{ij} were obtained from Ref. [21].

The total strains ε_{ij} can be calculated from the geometric equation

$$\varepsilon_{rr}=\frac{\partial u}{\partial r},\quad \varepsilon_{\varphi\varphi}=\frac{u}{r},\quad \varepsilon_{zz}=\frac{\partial v}{\partial z},\quad \varepsilon_{rz}=\frac{\partial u}{\partial z}+\frac{\partial v}{\partial r}, \tag{4}$$

where u and v are the displacement components in the radial and axial directions.

To solve these equations, the relationship between the total strains ε_{ij} and the elastic strains ε^e_{ij} needs to be known. Because the mechanical behavior of the silicon ingot at high temperature is not clear, three methods based on different material assumptions are introduced: the thermo-elastic method, the thermo-plastic method, and the thermo-creep method.

For the thermo-elastic method, the silicon material is assumed to be linear elastic, and the total strain is composed of two parts: the elastic strain and the thermal strain. The relationship between them is given by

$$\dot{\varepsilon}_{ij}=\dot{\varepsilon}^e_{ij}+\dot{\varepsilon}^T_{ij}, \tag{5}$$

where $\dot{\varepsilon}_{ij}$, $\dot{\varepsilon}^e_{ij}$, $\dot{\varepsilon}^T_{ij}$ are the total strain rate, the elastic strain rate and the thermal strain rate, respectively. The thermal strain rate is given by

$$\dot{\varepsilon}^T_{ij}=\alpha\dot{T}\delta_{ij}, \tag{6}$$

where α is the thermal expansion coefficient, which is given by [9]

$$\alpha=3.725\times10^{-6}(1.0-\exp(-5.88\times10^{-3}(T-124.0)))+5.548\times10^{-10}T. \tag{7}$$

In this method, the von Mises stress (σ_{von}) is used as the evaluation parameter for the silicon ingot:

$$\sigma_{\text{von}}=\sqrt{\frac{3}{2}S_{ij}S_{ij}}, \tag{8}$$