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Gas flow optimization during the cooling of multicrystalline silicon ingot

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ABSTRACT

Multicrystalline silicon (mc-Si) produced by unidirectional solidification system is a crucial photovoltaic material due to its relatively high conversion efficiency and low cost. Defects related to thermal stresses, for example, dislocation, significantly affect the performance of the material. In the paper, a global transient model is applied to examine effects of gas flow on stress levels inner the silicon ingot during the cooling process. The maximum von Mises stresses under different inlet gas velocities are presented as a function of the cooling time. Stress level with a high inlet velocity at the initial cooling is slightly lower, but is much larger at the late cooling than that with a slow velocity. An optimized condition with variable gas velocities at the inlet is proposed to improve the quality of silicon ingot by reducing the stress level during the cooling process.

1. Introduction

Recent years have witnessed impressive progress of the production of multicrystalline silicon (mc-Si) by the unidirectional solidification technique. However, silicon grown by this method has a relatively high dislocation density that reduces the minority carrier lifetime [1] and lowers photovoltaic conversion efficiency. Thermal stresses caused by inhomogeneous temperature field play an important role in generation and multiplication of dislocation during the solidification and cooling processes [2,3]. According to the theory [4], dislocations are easily generated inner the ingot where the effective stress exceeds the critical resolved shear stress (CRSS).

Many researches on the stresses in silicon ingot have been carried out [5–13]. Chen et al. [5] used a transient and global model to study the thermal stress distribution in the silicon ingot for different solidification time, as well as the effect of crucible constrains. They suggested that a longer solidification time and lower constrains should be adopted for growing a silicon ingot with low thermal stress and low dislocation density. Takahashi et al. [6] investigated the generation mechanism of dislocation, and found that dislocations come into being at grain boundaries and propagated as crystal growth proceeds. Moreover, the shear stress on the slip plane around the grain boundary is likely the cause of dislocation formation. Fang et al. [7] performed parametric studies to discuss the effect of furnace design on the interface shape and on the maximum von Mises stress. They concluded that the decrease of side insulation thickness, gas flow rate and distance from the bottom insulation to the heat exchanger block, as well as the increase of the top insulation thickness help to achieve a flat or slightly convex interface and the reduction of the maximum stress level and dislocation density in the growing ingot. Chen et al. [8] further studied the effect of thermal conductivity of a crucible on thermal stress and dislocations during the solidification using a three-dimensional global model, and concluded that temperature gradient in a silicon ingot as well as the melt-crystal interface shape should be controlled to reduce thermal stress and dislocations in a silicon ingot. Nakano et al. [9] considered the influence of the cooling rate on the dislocation density in mc-Si ingot during the unidirectional solidification process. They indicated that the maximum value of dislocation density decreases and that of residual stress increases with a fast cooling process. Zhou et al. [10] proposed a simplified model of dislocation density, and improved the traditional cooling process in the directional solidification of mc-Si. Their results showed that the final dislocation density could be reduced to about one fifth of that formed in normal cooling process. Wang et al. [11] built up a global transient model to study the effect of bottom insulation on thermal stress distribution in the mc-Si ingot during the cooling process, and found that the maximum von Mises stress is affected significantly by the insulation motion. In addition, generation and multiplication mainly occurs at the early cooling stage, and the lower part of the ingot always has no excessive stress, which means the region may have the best crystal quality. Zhao et al. [13] employed three methods to

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perform a quality assessment of silicon ingots produced in a directional solidification furnace. They concluded that the evaluation method based on thermo-elastic theory is preferred for efficient calculation in solidification process, and that for the whole solidification and annealing processes, the thermo-plastic theory and the thermo-creep theory are more suitable. They also found that large dislocation density is generated in the ingot during the annealing process.

Although investigations on thermal stress distribution in multi-crystalline silicon ingot have been conducted, there are few reports regarding the effect of gas velocity on the thermal stress during the cooling process. The main objective of the paper is to analyze the effect of the different gas velocities at the inlet on the cooling process, to present the relationship between the maximum von Mises stress and the gas velocities, and to propose an optimized gas inlet profile for the improvement of the crystal quality by reducing thermal-induced stress.

2. Problem description and mathematical models

2.1. System configuration

Schematic diagram of a typical directional solidification system is presented in Fig. 1. During the cooling process, the system components remain stationary except the bottom insulation that moves down directionally with a corresponding ramping-down of the heater power. To simplify the calculation, the heater power change is represented by a nonlinear temperature profile as described in Ref. [11]. The dimension of silicon ingot is 275 mm × 880 mm × 880 mm. The furnace information can also be found in Refs. [7,12]. The applied temperature profile along the heater and the motion of the bottom insulation are presented in Fig. 2. Thermal stresses generate during the solidification, release partially through the annealing, and pile up again during the cooling. The minimization of stress-related defects by reducing thermal stress has been an effective way to improve the crystal quality. In the actually industrial production, the silicon ingot is cuboids, and a three-dimensional model is required for an accurate analysis. However, the calculation time exceeds acceptance for an efficient study with the three-dimensionally transient model coupled with thermal field, flow field, stress field, and the tracking of the moving boundary due to the motion of the bottom insulation. Hence, a two-dimensional model, as applied in the Refs. [7,11], is adopted to save the computational load for a transient analysis of the cooling process.

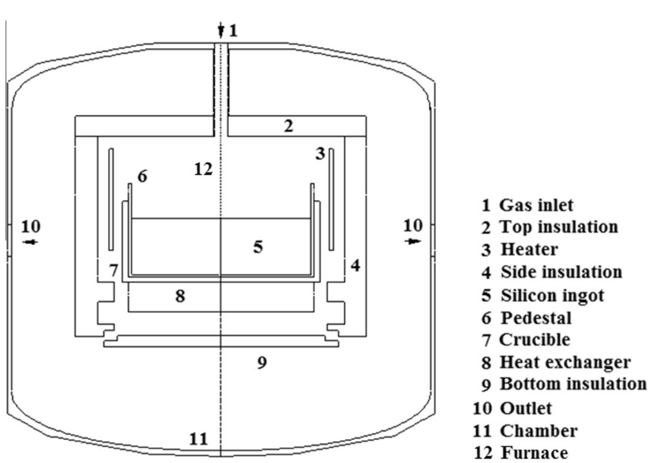

Fig. 1. Schematic diagram of a directional solidification furnace.

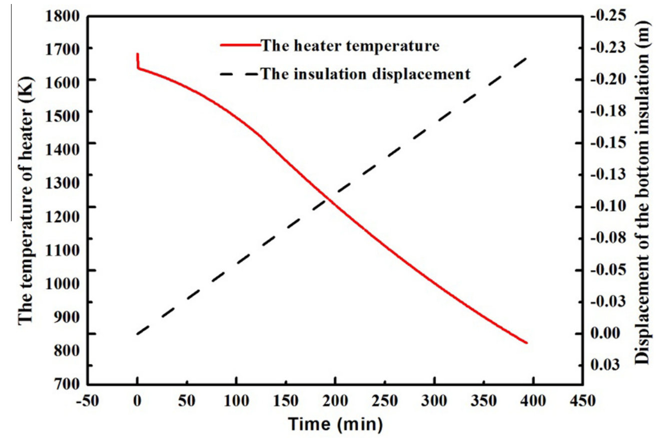

Fig. 2. The applied temperature profile on the heater and the motion of the bottom insulation during the cooling process.

2.2. Mathematical models

In order to get the distribution of thermal stress inner the silicon ingot, energy conservation equation is solved by coupling with the incompressible N–S equation. Gas velocity at the inlet is less than 0.6 m/s, which makes a maximum value of Reynolds number less than 440. Therefore, the gas flow can be treated as laminar flow. The following assumptions are further applied: (1) all the components in the chamber are diffuse-gray body; (2) the Boussinesq approximation is used to solve natural convection. In order to make the approximation applicable, the inlet can be set at the top insulation, where the gas is heated up, to limit the temperature difference of the gas; (3) the gravity is negligible compared to the thermal stress in the stress balance equations. The governing equations can be written as

$$\nabla \cdot \vec{\boldsymbol{u}} = 0, \tag{1}$$

$$\rho\frac{\partial \vec{\boldsymbol{u}}}{\partial t} + \rho(\vec{\boldsymbol{u}}\cdot\nabla)\vec{\boldsymbol{u}} = \rho\nabla(\nu\nabla\cdot\vec{\boldsymbol{u}}) - \nabla p - \rho_0\vec{\boldsymbol{g}}\beta_T(T-T_0), \tag{2}$$

where t is time, $\vec{\boldsymbol{u}}$ is velocity vector, and ρ_0 is the reference density; $\vec{\boldsymbol{g}}$ is the gravitational acceleration vector, β_T is thermal expansion coefficient of the fluid, and T_0 is the reference temperature ρ and ν are density and kinetic viscosity of the fluid, respectively. Temperature field is achieved by solving the energy conservative equation as

$$\rho_i C_{p,i}\frac{\partial T}{\partial t} + \rho_i C_{p,i}\nabla\cdot(T\vec{\boldsymbol{u}}) = \rho_i C_{p,i}\nabla\cdot(\alpha_i\nabla T) + \nabla\cdot q''_{r,i}, \tag{3}$$

where the subscript i indicates the components of the furnace; α_i and Cp, i represent thermal diffusivity and specific heat of the material at the ith domain, respectively; $q''_{r,i}$ is the radiation source term. Thermal stress is calculated by

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

$$\frac{1}{r}\frac{\partial}{\partial r}(r\sigma_{rz}) + \frac{\partial}{\partial z}(\sigma_{zz}) = 0, \tag{4}$$

where σ_{rr}, $\sigma_{\varphi\varphi}$, and σ_{zz} are normal stresses in the radial, azimuthal and axial directions, respectively, and σ_{rz} is shear stress. The stress–strain relationship is required to solve the above equation. For anisotropic thermo-elastic solid body it is taken as:

$$\sigma_{ij} = C_{ijkl}\left[\varepsilon_{kl} - \beta_{ij}(T - T_{ref})\delta_{kl}\right], \tag{5}$$

where σ_{ij}, ε_{kl} and δ_{kl} are stress tensor, strain tensor, and Kronecker delta tensor, respectively. β_{ij} is thermal expansion coefficient, and