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Process parameters influence on the growth rate during silicon purification by vacuum directional solidification

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ABSTRACT

A numerical model is proposed to investigate influences of process parameters, including crucible pulling down rates and heater temperature, on crystal growth rates for silicon purification by vacuum directional solidification. The crystal growth rates of a silicon ingot are analyzed based on the interface energy balance equation combining with the temperature field calculated by software of ProCAST, and the segregation behavior of impurities is investigated with the Scheil's equation. The results show that the crystal growth rates decrease linearly with the increase of heater temperature at a fixed value of the crucible pulling down rate, and increase exponentially with the increase of the crucible pulling down rates at a fixed value of the heater temperature. The numerical model is verified by removal of iron impurity from 300 ppmw to 1 ppmw and by the temperature of melt silicon which is recorded by a thermocouple. The results show that numerical results agree well with experimental results. This research is used for adjusting process parameters to control crystal growth during silicon purification by directional solidification.

1. Introduction

Multi-crystalline silicon, which accounts for more than 60% of the greatly increasing photovoltaic market [1–3], has triggered extensive efforts [4–7]. Directional solidification (DS) is an environmental friendly and inexpensively way for silicon production [8]. Crystal growth rate is an important factor for DS process because it significantly influences segregation behavior of impurities in silicon ingots, and then influences solar cell performances. Therefore, precisely controlling crystal growth rates are in favor of improving the purifying effect in silicon purification process.

Controlling crystal growth rate by process parameters includes the crucible pulling down rates and the heater temperature. The experiments have been confirmed that crystal growth rates increase with the increase of crucible pulling down rates, and decreases with the increase of heater temperature [9–12]. Further investigations suggested crystal growth rate was determined by heat flux flowing through solid–liquid interface of a silicon ingot [13]. During the DS process, silicon, as well as the crucible, moves downwards gradually from the hot zone to the cold zone. The increasing of crucible pulling down heights leads to larger heat dissipating area at the bottom of silicon. Herein more heat flux passes through the solid–liquid interface. However, the heat flux can't be measured directly by experiments. Namely, the detailed influence of process parameters on the crystal growth rates is still unclear. The purifying effect can be improved with a proper crystal growth rate in silicon production process. Thus, it is necessary to investigate the influence of process parameters on crystal growth rates. As we all know, the crystal growth rate is mainly influenced by temperature field. However, the temperature field is difficult to obtain by experiments. Fortunately, numerical simulation is an effectively way to investigate the temperature fields. So, the influence of process parameters on crystal growth rate is investigated with numerical simulation and experiments in this research.

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2. Numerical model

2.1. Model description

The configurations of the utilized vacuum industrial-scale furnace are shown schematically in Fig. 1. As is shown in Fig. 1(a), the major domains are labeled. In the furnace, the silicon material is loaded into a cylindrical crucible with 810 mm diameter and 290 mm height. Suitable crystal growth rates are controlled by adjusting heater temperature (T_h) and crucible pulling down rates (v_p). Redundant heat is eliminated by the furnace wall with cooling water and the cooler plate under the bottom of crucible. Maintaining the net heat flux over the solid–liquid interface is in favor of generating a vertical, homogeneous, columnar grain structure. Fig. 1(b) shows computational grids of DS furnace for silicon production, in which the computation domains were divided into six cell zones. For the purpose of saving computational resources, the furnace geometry was reduced to one-sixth and sixfold symmetry was applied. Temperature fields of the furnace were simulated by unstructured tetrahedral meshes which used 793239 cells. Element size was 0.01m, and mesh type was set as CTETRA 10. In the model, tetra aspect ratio and jacobian ratio were used to evaluate the quality of grids. The tetra aspect ratio was 8, and the maximum value of jacobian ratio was 0.8. The numerical model is set up based on the following assumptions: the geometry of the furnace model exhibits rotational symmetry, the physical properties of silicon are isotropic and functions of temperature, the melt is Newtonian fluid, and radiative transfer is modeled as diffuse-gray surface radiation.

2.2. Mathematics basis

For the mathematical model, the time–dependent temperature distribution is computed through the finite element method with the energy conservation, momentum and mass conservation equations. The transient temperature field of the silicon during the solidification process is calculated with the following energy equation [14].

$$\frac{\partial}{\partial t}(\rho H) - \nabla(\rho v H) = \nabla(K\nabla T) + S_T, \tag{1}$$

where t is time, ρ is density, H is the enthalpy of the material, ∇ is Hamiltonian operator, v is the velocity, K is thermal conductivity, T is absolute temperature and S_T is heat source. H can be expressed as:

$$H = h + \Delta H \tag{2}$$

where h is sensible enthalpy. ΔH is related to the liquid fraction of the solid–liquid interface, as is shown in Eq. (3).

$$\Delta H = \beta L, \tag{3}$$

where L is the latent heat. Liquid fraction, β, can be obtained as

$$\beta = \begin{cases} 0 & T < T_s \\ \dfrac{T - T_s}{T_l - T_s} & T_s < T < T_l \\ 1 & T > T_l \end{cases}, \tag{4}$$

where T_l and T_s denote liquidus temperature and solidus temperature, respectively.

The velocity of liquid is provided by the momentum equation [15].

$$\frac{\partial u}{\partial t} = -\frac{1}{\rho_0}\nabla p + \frac{\rho - \rho_0}{\rho_0} g + \mu \nabla^2 v, \tag{5}$$

where g is the gravitational acceleration, μ is the molecular kinematic viscosity, ∇^2 is the Laplace operator, ρ is the density and ρ_0 is the reference density.

The mass conservation equation must also be satisfied.

$$\frac{\partial \rho}{\partial t} + \nabla(\rho v) = 0 \tag{6}$$

The irradiation flux in furnace can be calculated as

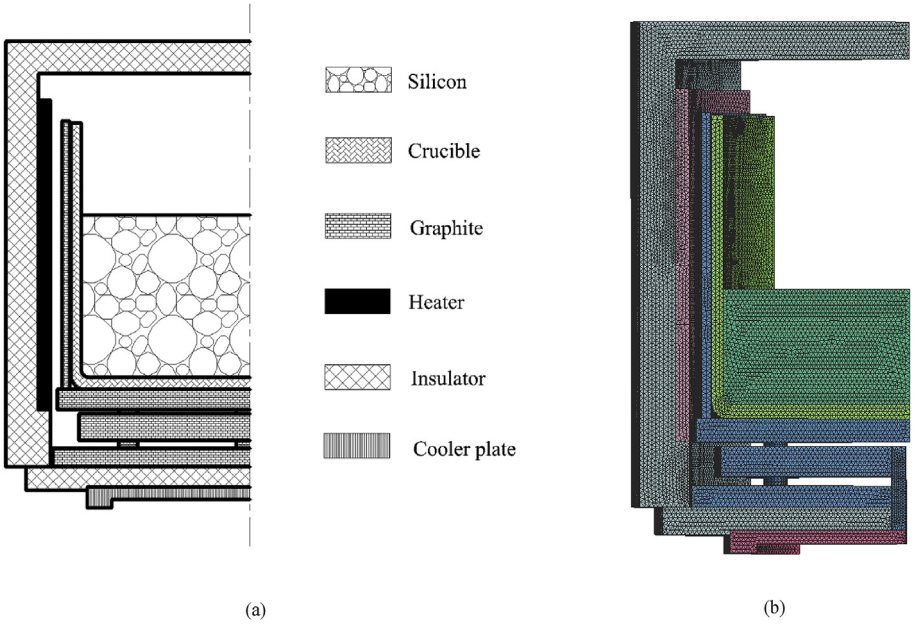

Fig. 1. Schematic of the DS furnace model: (a) configurations; (b) computational grids.