Journal of Crystal Growth 381 (2013) 169–178

Contents lists available at ScienceDirect

Journal of Crystal Growth

journal homepage: www.elsevier.com/locate/jcrysgro

Numerical parameter studies of 3D melt flow and interface shape for directional solidification of silicon in a traveling magnetic field

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ARTICLE INFO

Article history:
Received 14 March 2013
Received in revised form
23 May 2013
Accepted 20 June 2013
Communicated by J.J. Derby
Available online 11 July 2013

Keywords:
A1. Computer simulation
A1. Fluid flow
A1. Magnetic fields
A2. Directional solidification
B2. Multicrystalline silicon

ABSTRACT

The role of various growth and process conditions (Lorentz force, temperature gradients in the melt and the crystal, steady-state crystallization velocity) in directional solidification of multicrystalline silicon in a traveling magnetic field is analyzed for a research-scale furnace (melt size of $22 \times 22 \times 11$ cm^3). The influence on the melt flow pattern, the typical melt flow velocity, the oscillation amplitude of the velocity and the temperature, the shape of the crystallization interface is determined using three-dimensional (3D) numerical calculations with the STHAMAS3D software and a local quasi steady-state model. It was found that both the interface shape and the melt flow are sensitive to the variation of the considered growth and process parameters.

1. Introduction

Directional solidification of large multicrystalline (mc) silicon ingots is one of the main methods for the production of photovoltaic silicon. Although the corresponding crystallization furnaces may have a very complex construction, the key processes determining the ingot quality occur locally at the crystallization interface. From a macroscopic point of view, the interface is described by its shape and the crystallization velocity, which are determined only by a few growth parameters: the temperature gradient in the melt, the temperature gradient in the crystal, and the melt flow conditions. The temperature gradients can be controlled by the furnace design and the thermal process. An active control of the melt flow is possible using time-dependent magnetic fields, for example, a traveling magnetic field (TMF) [1]. This gives the crystal grower additional process parameters such as the inductor current and the direction of the TMF. A deep understanding of the influence of the growth and process parameters on the crystallization interface is crucial for the optimization of the ingot quality.

Numerical modeling can be very useful for both the physical understanding of the process and the optimization of the experimental equipment. Several works are devoted to the influence of the melt flow on the interface shape for the directional solidification of silicon in the so-called quasi steady-state approximation [2–8]. This approach assumes that for interface positions in the middle part of the melt height, the thermal conditions on both sides of the interface (in the crystal and in the melt) remain approximately constant over time intervals long enough to allow the changes in the interface shape to develop [1]. This assumption implicates that the reaction time of the interface shape on the changes in the melt flow is smaller than the total solidification time.

The quasi steady-state approach requires the specification of an average crystallization velocity, which sets the released latent heat. Appropriate thermal conditions in a local or a global furnace model and/or the pinning of some interface points ensure that the interface remains in the middle part of the melt. Global models of different degrees of complexity have been presented in the literature [3–6]. However, local models are still useful for a fundamental understanding of the sole influence of a single growth parameter on the melt flow and the interface shape. A local three-dimensional (3D) model containing only the melt and the crystal, with a fixed temperature distribution and a given crystallization interface position at the inner side of the crucible wall has been applied, e.g., in [2,7,8].

This paper continues the study of directional solidification of silicon in a research-scale furnace in a TMF, which corresponds to the geometry of the so-called Generation 1 crucible

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http://dx.doi.org/10.1016/j.jcrysgro.2013.06.023

($22 \times 22 \times 22$ cm^3) presented in [1], but uses the quasi steady-state approach to carry out comprehensive 3D parameter studies. A local model for the melt and the crystal based on the STHAMAS3D code is applied following the previous works for directional solidification of silicon [2,7,8]. It is the aim of this paper to look closer at the influence of the intensity of a TMF, the temperature gradient in the melt, the temperature gradient in the crystal (the crystallization velocity in the quasi steady-state approach) on the melt convection and the interface shape.

2. Numerical model

2.1. Melt flow and crystallization

The computational domain used for the local 3D simulations of the heat transport consists of the silicon melt and the silicon crystal only. The melt flow is described by the 3D equations of mass, momentum, and heat transport. For an incompressible Newtonian fluid in a Cartesian coordinate system, the equations for the flow velocity $\vec{u}$, the pressure p, and the temperature T take the form,

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

$$\rho\left[\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u}\right] = -\nabla p + \eta\Delta\vec{u} + \vec{F}_L - \beta(T-T_{ref})\rho\vec{g}, \tag{2}$$

$$\rho c_p\left[\frac{\partial T}{\partial t} + (\vec{u}\cdot\nabla)T\right] = \lambda\Delta T, \tag{3}$$

where ρ is the fluid density, η is the dynamic viscosity, c_p is the heat capacity, λ is the thermal conductivity. The symbols β, T_{ref}, and $\vec{g}$ denote the coefficient of thermal expansion, the reference temperature, and the gravity vector, respectively, within the Boussinesq approximation for the buoyancy forces. The Marangoni forces are neglected in this study because their influence is limited to a region near the free surface [2]. $\vec{F}_L$ is the time-averaged density of the Lorentz force generated by the applied TMF.

The open source finite element package GetDP is used to compute the time-averaged spatial distribution of the Lorentz force density in the melt by solving the time-harmonic 3D equations for the electric scalar potential and magnetic vector potential; see [1,9] for further details. The Lorentz force distribution is then imported into STHAMAS3D and is considered constant during the whole computation. We have estimated that due to changes of interface shape or position, the Lorentz force density or the force angle with the horizontal plane may change by less than 20%. The geometry is identical to that in [1] and consists of three TMF inductors and a silicon melt as shown in Fig. 1(a). The cross section of the inductors is 2×8 cm^2, the distance between inductors is 2 cm, and the distance to melt is 8 cm. The bottom of the melt is located 2 cm below the horizontal mid-plane of the inductors. At the center of one side ($x > 0$), there are current supplies with a gap of 2 cm. The frequency of the alternating current is set to 50 Hz. The eddy currents are computed only in the silicon melt (electrical conductivity of 10^6 S/m). Fig. 2(b) shows the calculated Lorentz force distribution for the reference case with an inductor current of 300 A and an upward TMF (with a phase shift of 60°). A downward TMF basically reverses the vertical component of the Lorentz force; the entire force distribution scales with the square of the inductor current.

At the crystallization interface, the latent heat generation is considered for a prescribed steady-state crystallization velocity v_g,

$$\lambda_S \nabla T|_S \vec{n} - \lambda \nabla T|_L \vec{n} = v_g \rho_S q_0, \tag{4}$$

where λ_S and ρ_S are the thermal conductivity and the density of solid silicon, respectively, and q_0 is the latent heat; the normal vector points into the melt. To determine the position and the shape of the crystallization interface, a phase tracking procedure is used. The crystallization interface is the block boundary between the solid and the liquid block. The finite volume method is used to solve the temperature equation on the entire block-structured mesh, and the boundary condition on the crystallization interface is iteratively applied in the form of Eq. (4). In every iteration, there is a data exchange between the solid and the liquid block. The grid is relaxed when deformed in Oz direction in accordance with the following procedure:

$$z_{new} = z_{old} + c(z_{iso} - z_{old}),$$

where z_{new} is the new coordinate of the point at the block boundary between the solid and the liquid, z_{old} is the old coordinate, z_{iso} is the coordinate of the point where the vertical line of the point at the block boundary intersects the melting point isotherm, and c is a relaxation factor. We used $c = 0.3$–0.5, but decreased it to $c = 0.01$ for the case with the highest TMF inductor current. High values of c can introduce numerically instabilities and thus can be used only for flow conditions that are close to a quasi steady-state. Normally, we obtained a precision between 0.1 K and 0.25 K for the temperature difference between the block boundary and the isosurface of the melting temperature. This temperature difference corresponds to a distance between 1 mm and 2.5 mm for a temperature gradient of 1 K/cm in the melt.

The time-dependent computations were performed with the finite volume code STHAMAS3D, which has been already used for solving convective heat and mass transfer problems in directional solidification [2] and Czochralski configurations [10]. The SIMPLE algorithm is applied for the pressure correction, and the implicit Euler method is applied for the time integration. At every time step, the convergence criteria for SIMPLE iterations are set to decrease the residuals of the pressure correction equation by four orders of magnitude. Normally, 25–30 iterations are necessary. A flux blending between the central differencing scheme (CDS) and the upwind differencing scheme (UDS) is used for the convective fluxes. In the present simulations, we have used a flux blending of 80% CDS along with UDS. A higher percentage (~100%) of CDS may cause a numerical instability when high-frequency turbulent fluctuations occur. A lower percentage of CDS (~0%) will suppress mechanical instabilities due to the numerical diffusion. It has been shown by measurements in model melts in [9] that a CDS can be used to calculate unsteady 3D flows in a TMF also without explicit turbulence models. The Reynolds number in the current study reaches approximately 6000 at a flow velocity of 16 mm/s.

The computational block-structured, non-orthogonal grid is subdivided into two blocks (for the melt and the crystal) with a local grid refinement at the surfaces to resolve the boundary layers. In the reference case, the entire grid consists of 350,000 nodes; there are 50 nodes in the Ox and Oy directions and 140 nodes in the Oz direction. In the melt, the size of the first control volume (CV) is 0.7 mm at the crystallization interface, 1.8 mm at the side walls, and 0.4 mm at the free surface. The second CV is twice larger, and the following CVs at the three different surfaces grow in a geometric progression with factors of 1.007, 1.02, and 1.04, respectively. The grid is similar in the crystal except a refinement at the crystallization interface (initial size of 0.05 mm and growth factor of 1.06).

To obtain a realistic time-average solution starting from an arbitrary initial state, at least 1200 s of real time were computed with a time step of 0.1 s. The last 500 s were used to compute a time-averaged solution. Therefore, a high computational power is needed to perform a parametric study under these constraints. The 3D time-dependent simulations were performed on a HP-AMD-Opteron 2.2 GHz cluster (1 Gbit/s switched) with the