TRANSIENT MODELING OF FZ CRYSTAL GROWTH PROCESS AND AUTOMATIC ADJUSTING OF THE HF INDUCTOR CURRENT AND FEED ROD VELOCITY

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Introduction. Nowadays, the modern industrial floating zone (FZ) growth process allows the production of single-crystalline silicon rods up to 200 mm in diameter. This progress in the growth technique needs support by the numerical modeling to enhance the product quality, save resources and to improve the control of the processes in the FZ growth facility. Numerous 2D (i.e., axisymmetric) computational studies have been made to investigate the FZ crystal growth in the steady-state approximation (e.g., [1]–[3]). However, only some of them consider the modern industrial FZ growth with a high-frequency needle-eye inductor and do undertake the full modeling of the phase interfaces and free surface shape. A very precise model for complete steady-state calculation of the phase boundaries for large industrial FZ silicon crystal growth by the needle-eye technique is described in [4].

Various important FZ processes features have a time-dependent character and can be studied only with the help of a fully transient model. Therefore, from the steady-state model we have developed a fully transient model and a corresponding program package FZoneT in [5]. This transient approach allows studies of such substantially time-dependent process phases as the growth of the starting and ending cones of the crystal rod, which is especially very important for the growth of large crystals in practice. In the present paper we describe the summary of the transient numerical approach and the underlying models as well as some new calculation results including: 1) verification of the mass control in the transient model; 2) investigation of FZ system's response to small alternations of the process parameters; 3) automatic control of the crystal growth by a set slope angle.

1. Summary of transient modeling of FZ process. The transient model is based on further development of the models which were proposed in [4] for steady state calculations: 1) models for the open melting front of the feed rod, melting and crystallization interfaces; 2) a model for calculating a high frequency (about 3 MHz) electromagnetic field induced by a slotted pancake inductor; 3) a steady-state model for calculating the geometry of melt free surface and the position of the inner triple point; 4) a model for heat exchange calculation due to radiation (accounting for view factors); 5) a transient model for diffusive heat transfer in all silicon parts (feed rod, melt and single crystal).

Additionally, for the modeling of the FZ process fully in time, the silicon volume control in the molten zone has to be carried out. This volume control coupled with free melt surface calculation enables to model changes of the crystal radius in time (for details see [5]).

1.1. Control of the mass conservation in the FZ system by controlling the volumes in the melt and solids. In Fig. 1*a* the scheme for transient FZ modeling is shown. The most important aspect of transient modeling for the FZ process is

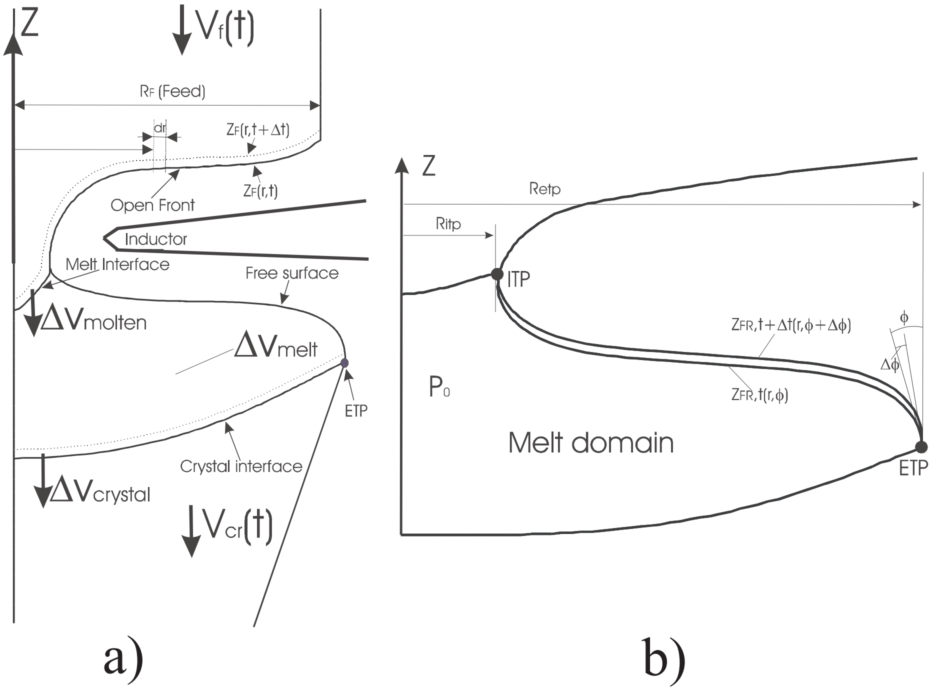

Fig. 1. (*a*) FZ system, transient calculation of volumes; (*b*) free melt surface calculation.

the control of the mass conservation in the melt and in solid silicon parts. The feed pushing rate $V_F(t)$ and the crystal pull rate $V_{CR}(t)$ are considered as time dependent values. Thus the shape of the molten zone and consequently the actual crystal radius can be time-dependent, too.

In Fig. 1*a* ΔV_{molten} indicates the molten volume of silicon during a time interval Δt, which flows from the feed rod into the melt domain; $\Delta V_{crystal}$ is the loss of melt volume because of the crystallization process at the interface with a single crystal for the same time interval; ΔV_{melt} is the total change of volume in the melt domain due to the values of ΔV_{molten} and $\Delta V_{crystal}$. Thus, the volume conservation law gives: $\Delta V_{melt} = \Delta V_{molten} - \Delta V_{crystal}$ (for details see [5]).

1.2. Relation between the melt volume change and the free melt surface shape and crystal radius. It is clear that within a short time interval Δt with fixed melt and solid silicon interfaces, the melt volume change ΔV_{melt} causes the change of the melt free surface Z_{FR}(r,t) (see Fig. 1*b*), where ITP (internal triple point) and ETP (external triple point) are the endpoints of the free surface. Hence during calculations the melt free surface must be adjusted so that the change of melt volume matches with the expected change ΔV_{melt}.

Knowing the positions of the triple points (ETP and ITP) and the angle ϕ (an angle between the vertical axis and the tangent of the free surface at ETP) it is enough to define the shape of the melt free surface Z_{FR}(r,t) by requiring that for every point the capillary, hydrostatic, electromagnetic and gauge pressures are balanced on the free surface. Consequently, the melt free surface for the given time instant t can be considered as a function from the parameter ϕ, i.e., $Z_{FR,t}(r,\phi)$. The new shape of the free surface is found by an iterative recalculation with different angles ϕ, trying to match the actual volume of the melt. Using this approach in transient modeling is justified by a relatively fast change of the free surface with respect of other phase boundaries.

The change of the crystal radius during transient modeling is governed by the

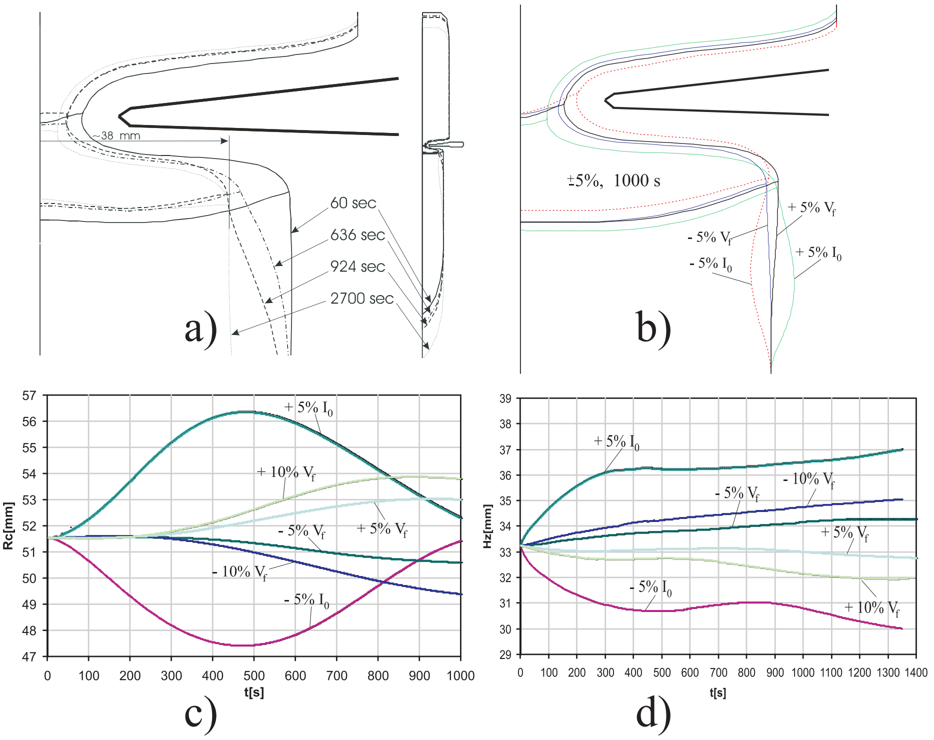

Fig. 2. (*a*) Shapes of phase boundaries at various time instants after the decrease of V_F; (*b*) changes in phase boundaries of the FZ system due to 5% alternations of I_0 or V_F at 1000 sec since start; (*c*) crystal radius response to 5% and 10% alternations of I_0 and V_F; (*d*) zone height response to 5% or 10% alternations of I_0 and V_F.

actual value of the angle ϕ (angle with a vertical axis). In the reference system attached to the single crystal, the new position of ETP in a time instant $t + \Delta t$ is found as a intersection point of the tangent of the free surface at ETP in a time instant t with the tangent of the crystallization interface at ETP in a time instant $t + \Delta t$ (for details see [5]).

2. Examples of calculations for transient processes and for automatic adjusting. Presented calculations are carried out for a 4" FZ crystal growth system described in [5]. The base value of the inductor current was I_0 = 970 A and the feed rod velocity V_F = 1.538 mm/min. First, the crystal radius response to a decreased feed rod pushing rate is investigated. In the steady-state, the crystal radius R_{CR} must obey the following equation regarding mass conservation: $V_{CR} \cdot R_{CR}^2 = V_F \cdot R_F^2$, where V_{CR} is the crystal pulling rate; V_F is the feed rod pushing rate; R_F is the feed rod radius. If the feed rod pushing velocity V_F is decreased, then the new equilibrium radius R_{CR} will be smaller. This is illustrated by a calculation example in Fig. 2*a*, where at the equilibrium state, V_F = 1.538 mm/min (R_F = 65 mm, V_F=2.45 mm/min) is instantly decreased to V_F = 0.837 mm/min. The resulting crystal radius has reached its new equilibrium value approximately in 2700 sec and agrees well with the mass conservation equation.

The calculations of the response of the FZ system to small instantaneous changes ±5%, ±10% of the inductor current I_0 or feed rod velocity V_F are illustrated (Fig. 2*b*,*c*,*d*). The response of the system is shown for two parameters: the crystal radius R_C and the zone height H_Z (vertical distance from ETP to the outer rim of the feed rod). The calculated shapes of the system at 1000 sec after change instant are shown in Fig. 2*b*. Fig. 2*c*,*d* show R_{CR} and H_Z dependencies on

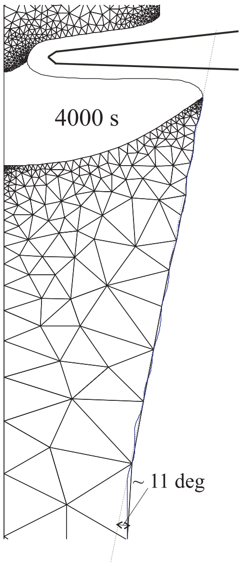

Fig. 3. Numerically calculated process with automatic regulation for V_F and I_0 that ensures the crystal growth with the given slope angle of 11 degrees, phase boundaries and FEM mesh during 4000 sec since start.

the time.

To ensure the crystal growth with a constant slope, the automatic regulation based on the PID algorithm (proportional integral differential algorithm) for I_0 and V_F is implemented in FZoneT. During regulation, I_0 and V_F are adjusted depending on the deviation of the actual and desired values for the slope of the crystal surface and zone height. The constants in the PID algorithm are chosen according the gathered experience in a previous calculation sample. The calculation sample in Fig. 3 shows the modeled crystal growth process with a desired slope angle approximately of 11 degrees.

3. Conclusions. 1) A fully transient system of models has been developed for calculating phase boundaries in large industrial FZ silicon crystal growth by the needle-eye technique. The implementation of transient models in the computer program FZoneT has been done. 2) The calculation samples in this paper show that the presented transient approach allows studies of such substantially time-dependent process phases as the automatically regulated growth of the starting and ending cones of the crystal rod which is especially very important for the growth of large crystals in practice.

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