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Crystal twisting in Cz Si growth

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ABSTRACT

Crystal twisting during Czochralski growth of silicon crystals is sometimes observed at increased pulling rates. Crystal twisting with spatial fluctuations of the crystal surface and diameter may result in losing growth control or in the need of lowering the pulling speed. There are many ideas in the literature about reasons of spiral growth or twisting during Cz crystal growth of oxides and other materials. We contribute to this research, analyzing large scale Cz Si growth. For varying growth conditions, we have observed correlation between melt supercooling over the free surface and the start of crystal twisting. These findings support the idea that crystal twisting is closely related to a temperature distribution along the melt free surface near the tri-junction point. Correlations of melt supercooling with crystal twisting have favored developments of a predictive criterion of crystal twisting, which can be used to find the maximal stable crystallization rate by computer modeling for a particular hot zone design.

1. Introduction

Industrial Czochralski growth of silicon crystals is the main technique to manufacture from 100 to 300 mm diameter wafers for integrated circuits used in computers, mobile phones, and a wide variety of other electronic devices, including solar cells. Crystal twisting or spiral like growth of Czochralski silicon crystals may be observed at increasing pulling rates as an undesirable phenomenon decreasing the yield of production. If the pulling rate reaches a high critical level, the smooth crystal side surface becomes wavy with a spiral like morphological structure along the ingot. There are examples of standard and twisted 300 mm diameter Cz Si crystals in Fig. 1a and b, respectively. Crystal twisting may result in losing control of the crystal diameter, which sometimes cannot be stabilized by a monitoring control system. The decrease of the crystal pulling rate is an effective tool to avoid twisting. However, the cost of production subsequently increases for a lower pulling rate. As well lowering the crystallization rate may result in self-interstitial rich crystal periphery, originating microdislocation loops at lowering temperature. So to understand and to avoid conditions of transition from cylindrical to spiral like crystal shape are of high importance for maximal performance of industrial crystal growth technology at maximal crystallization rates with optimal crystal quality and without surface instabilities.

A phenomenon similar to silicon twisting at final stage is known as spiral growth in crystallization of oxides. Takagi and Fukazawa [1] have examined different changes in heating conditions and Cz growth parameters with a conclusion that the BGO crystal shape can be improved by reducing the radiation heat loss from the melt free surface. Okano et al. [2] have revealed that $DyAlO_3$ crystals tend to twisted growth more frequently in comparison to more transparent $HoAlO_3$ and $ErAlO_3$ Cz crystals. Fei et al. [3] reported that spiral or twisted growth was the problem in Cz SGGG crystals, which could be overcome by raising the crucible position with respect to the RF heater, increasing the temperature gradient at the growth interface. Kamada et al. [4] discuss that the reason for twisting formation in Cz Pr:LuAG growth is asymmetric temperature distribution come from unstable melt convection. However, smooth shape growth of Pr:LuAG crystals was reported after modifications of many technological parameters and without evidences that melt convection become stable [4]. Melt flow instabilities as a reason of spiral growth and twisting are discussed in many other papers but this point of view is questionable because the time scales of hydrodynamics and crystal growth spirals are different in from three to five orders of magnitude. Schwabe et al. presented a detailed list of conditions favoring spiral growth of high melting point oxides available in the literature (see [5] and references within). As the most important factors of spiral growth Schwabe et al. mention the radiative heat transfer dominating over thermal conduction through the crystal and the small radial temperature gradients in the melt near the crystal.

We imply that general physical reasons of spiral growth and twisting of oxides should be applicable to Cz growth of silicon.

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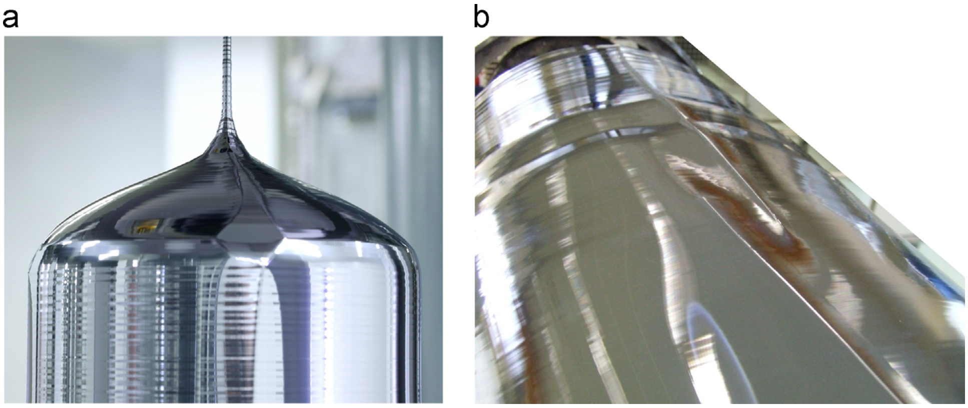

Fig. 1. Experimental photos of cylindrical (a) and twisted (b) Cz Si crystals of 300 mm diameter.

Details of heat transfer in the crystal and in Si melt can be comprehensively studied by computer modeling. We have used CGSim^{TM} software v.14 [6] developed by STR Group as a simulation tool in 2D and 3D, quasi-steady and unsteady approximations. Growth parameters and experimental data obtained in Siltronic AG were numerically reproduced to get better insight into crystal growth physics and to verify one criterion of crystal twisting, which we propose in the present paper.

2. Numerical model

Modeling of mass conservation and momentum exchange in and between the melt and gas flows is performed within the Navier–Stokes equations written in the approximation for slow subsonic gas motion, and extended by heat conservation equation and the view-factor method for simulation of radiative heat exchange [7–9]. For modeling of melt convection, the Boussinesq approximation is applied, where melt density is calculated as a linear function of the temperature. The Finite Volume (FV) method with high approximation orders is used for discretization of equations, allowing modeling of both diffusion and convective terms with up to 4th approximation accuracy order including integration of non-linear flux distributions over faces of a FV [9]. To simulate turbulent mixing in the melt, we have used a modification of the model of Wolfshtein [10] as described by Ivanov et al. [11]. The Wolfshtein turbulence model belongs to the family of *k–l* models in which only one model transport equation is solved for the turbulence kinetic energy.

3. Results and discussion

Experimental crystal growth and computer modeling used to research the twisting phenomenon have been performed in different Cz hot zones and crystallization systems to grow Si crystals with the diameters 100, 200, and 300 mm. As an example in Fig. 2a, there is a schematic view of EKZ 1300 system to grow 100 mm diameter Si crystals [7]. Stable crystal growth is experimentally provided in the system with the pulling rates up to 1.7 mm/min. Increasing the pulling rate to1.8 mm/min or higher (without changes of the hot zone design) usually resulted in crystal twisting.

Experimental data obtained for Cz Si growth of 100 mm diameter crystals were studied by detailed 3D unsteady computer analysis within the LES/RANS approach [8,11], including the initial stage of 2D quasi-steady global heat transfer (GHT) modeling [7] using CGSim software (see Fig. 2b and c). The computational grid for 2D GHT consisted of about 29,000 FVs including structured and unstructured blocks (see a fragment in Fig. 2b). 3D structured grid of 993,000 FVs suitable for the combined LES/RANS approach is presented in Fig. 2c, including the crystal, melt, crucible, and limited gas region. 3D unsteady calculations were performed with the time step of 0.125 s for the time period longer than 1300 s, which is sufficient to get a solution independent on transitional fluctuations and initial flow distributions. All physical properties of silicon and other materials were used as published before in [7,8].

Si melt flow can be described by several dimensionless parameters, estimating the effect of volume or surface forces on the viscous force. The Rayleigh number associated with natural convection in the melt is $Ra = 2 \times 10^7$. The Reynolds numbers estimated by the rate of crystal rotation and crucible rotation are, correspondingly, $Re_{crys} = 1.7 \times 10^4$ and $Re_{cruc} = 3.8 \times 10^4$. The Marangoni number regarded as the effect of thermal-surface tension is $Ma = 2.3 \times 10^4$. To describe the dynamical effect of Ar gas flow on the melt flow via the effect of the gas shear stress over the melt free surface [7], the following dimensionless number (*DN*) can be proposed [12]:

$$DN \equiv \frac{\tau_g H^2 \rho_l}{\mu_l^2} \quad (1)$$

The notations in Eq. (1) are the following: the length scale H of the surface affected by the gas shear stress, the surface-averaged shear stress scale τ_g generated by the gas flow, the melt density ρ_l and dynamic viscosity μ_l. For the crystal growth case presented in Fig. 1, the dimensionless number *DN* is equal to 2×10^6, which is nearly two orders of magnitude higher than the critical *DN* value of 5.13×10^4 [12] responsible for generation of unsteady fluctuations. Even for the *DN* value of 1.25×10^5 (which is one order of magnitude lower than *DN* in the current results of 3D Si melt modeling) the gas shear stress leads to generation of well-developed turbulence in the melt as demonstrated by the analysis of the power spectral density [12]. So the effect of natural convection and the effect of the gas shear stress are here the major forces governing turbulence in Si melt, representing heating and gas flow conditions.

Instantaneous temperature distributions over the melt free surface, obtained by 3D unsteady modeling, are illustrated in Fig. 3. One can see that the melt temperature is lower for the case of higher crystallization rate, which is related to a lower heater power. The main cooling effect on the melt free surface is related to radiative heat exchange with surrounding surfaces. Cooling of the melt due to the gas flow is of minor effect in comparison to radiation. Areas of super-cooled melt with the temperature lower than the melt/crystal interface temperature are located close to the crystal, displayed by violet color. It is evident that the supercooled areas are much larger for the case of the higher crystallization rate. After a reasonable time-averaging, the temperature distributions over the melt free surface should become axisymmetric and instant areas of supercooled melt may disappear. To get time-averaged results shown in Fig. 4, we used a time period of about 700 s. It is interesting that, for the case of the