To investigate interface shape and thermal stress during sapphire single crystal growth by the Cz method

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Global modeling is performed to predict electromagnetic field, heat transfer, melt flow, solid/liquid (S/L) interface shape, and thermal stress during RF-heated Czochralski (Cz) single crystal growth of sapphire. The relations between the convexity of the S/L interface and growth parameters, i.e., crystal rotation rate, crystal size, furnace insulation, and RF coil, are established. Thermal stress is represented by the von Mises stress, and the stress status in the growing crystal is characterized by the maximum von Mises stress. The curves regarding growth parameters and the maximum von Mises stress are obtained. According to the analysis, a flat or slightly convex S/L interface could be achieved by modifying the growth parameters, and the crystal quality could be improved by reducing thermal stress and its related defects.

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1. Introduction

Sapphire has wide applications in many areas, such as Silicon-on-Sapphire (SoS) for RF devices, lasers, optical windows, wearing and cutting tools [1], due to its high melting point of 2320 K, high hardness (ranking a 9 on Mohs’ scale), high chemical stability, and excellence in optical, mechanical and electrical properties. The latest booming of sapphire industry has been inspired by the rapid development of Light Emitting Diode (LED) devices, in which the c-plane (0001) sapphire works as a substrate for GaN thin-film crystal growth using the metal–organic chemical vapor deposition (MOCVD) process [2]. The most recent overview of the lastest market trends and modern competing methods of sapphire crystal growth, and the application of sapphire as LED substrates was presented by Akselrod and Bruni [3].

The primary focus of the current sapphire production is to massively produce large-size and high-quality crystals with low bubbles and low dislocation density. Although the Czochralski method [4] has virtually dominated the entire production of single crystals for microelectronic and optical industries [5], most crystals, currently, are grown by Kyropoulos or HEM methods rather than by Czochralski for the substrate application of GaN growth. The reason is the high dislocation density of the grown crystal. Therefore, it is critical to study the formation and multiplication of dislocation during the Cz-sapphire crystal growth to improve the crystal quality. Numerical simulations of high-melting point and semitransparent oxides have been conducted since the past decade. Budenkova et al. [6] studied the effect of internal radiation and reflection on the temperature fields and S/L interface in sapphire Cz growth. Tavakoli [7] predicted the flow and temperature field numerically using the finite element method for different stages of the Czochralski crystal growth of sapphire. Lu et al. [8] numerically investigated the effect of the RF coil position during the stages of sapphire crystal growth process in an inductively heated Czochralski crystal growth furnace on the thermal and flow transport, the shape of the crystal–melt interface shape, and the power requirements. Demina and Kalaev [9] presented 3D features of melt convection during sapphire crystal growth using both Cz and Ky methods. The major defects in the sapphire single crystals are dislocation and small bubbles, known as micro-voids . The possible mechanisms of bubble formation were reviewed [10,11]. Dislocation and cracking are two types of stress-related defects that significantly degrade the application of sapphire crystals [12,13]. Traditional theories [14–16] indicate that the regions with an intensive dislocation multiplication by comparing the von Mises stress with critical resolved shear stress (CRSS). Miyazaki and Okuyama [17] and Miyazaki et al. [18] applied the Hassen–Alexpander–Sumino model to predict dislocation density in a bulk single crystal, in
which creep strain rate is related to dislocation density. The von Mises stress can be used to represent the stress status in a crystal, and the reduction of its maximum value during crystal growth is a promising way for the minimization of dislocation density.

In the present paper, an integrated mathematical model [10] is applied to study heat transfer, fluid flow, interface shape and thermal stress distribution during a stable RF-heated Cz-growth process of sapphire single crystal. Parametric studies are conducted to achieve the relations between the convexity of the S/L interface and the growth parameters, and between the maximum von Mises stress in the growing crystal and the growth parameters. From the analysis, a flat or slightly convex interface shape, which is preferred for the growth of high-quality crystal, could be obtained by adjusting the furnace design and growth conditions.

2. Problem description and numerical method

2.1. Problem description

A schematic diagram of a Cz crystal growth apparatus is shown in Fig. 1. The system mainly includes an iridium crucible, a seed rod, double-layered ZrO₂-based heat insulation, crucible supporter, alumina vessel, a RF coil, and heater shield. The chamber of the furnace is in inert (N₂) or oxidizing atmosphere (N₂ + 2 vol% O₂), or in vacuum. The weight loss of the iridium crucible is inevitable during the Cz growth process, especially in oxidizing atmosphere, and the crucible life time is around 2 or 3 months. The charge weight of the raw material is about 6.5 kg, and the crystal weight is about 5 kg. The grown boule diameter is 2–5 in. with a plane orientation of the c axis. The total growing time varies from 2 days to 4 days, depending on the crystal size and the pulling rate. The stable growth stage, on which the present study focuses, is usually several days with an average power consumption of 30 kW.

2.2. Governing equations

The modeling is conducted for the stable growth stage of sapphire single crystal. The following assumptions are further made for the thermal and flow fields in the present model: (1) the system is in a quasi-steady state, and the furnace geometry is axisymmetric; (2) the natural convection could be solved using the Boussinesq approximation; (3) the internal radiation of the melt is neglected, while that of the crystal is treated by an artificially enhanced thermal conductivity [19]; with such a treatment, the crystal can further set as an opaque material during simulation; (4) the thermo-physical properties of the furnace are constant, and the melt is assumed as opaque [7]; (5) the free surface is assumed to be flat, i.e., the wetting of the melt on the iridium crucible is neglected. The Rayleigh number of the melt is approximated as 10⁷–10⁸ based on the crucible diameter around 0.22 m, the properties in Ref. [20] and a temperature difference of 100–200 K, which is less than the transition value to turbulence, 10⁹. Therefore, the melt convection can be considered as laminar flow. Based on the above discussion, the governing equations can be described as follows [10,20]:

\[ \nabla \mathbf{u} = 0, \]

\[ \frac{d\mathbf{u}}{dt} + \mathbf{u} \nabla \mathbf{u} = -\nabla p + \frac{\mu}{\rho} \nabla \times \mathbf{b} + \frac{1}{\rho} \nabla \left( \frac{g \beta}{T - T_0} \right), \]

where \( t \) is the time, \( \mathbf{u} \) is the velocity vector, \( \rho \) and \( \nu \) are the density and kinematic viscosity of the fluid, respectively, \( g \) is the gravitational acceleration vector, \( \beta \) is the thermal expansion coefficient of the fluid, \( T \) is the temperature, and \( T_0 \) is the reference temperature. The heat transfer equation is described as

\[ \frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{u} T) = \nabla \cdot \left( \kappa \nabla T \right) + \dot{q}_{\text{ed}} + \dot{q}_{\text{ir}} + \dot{q}_{\text{iso}} + \dot{q}_{\text{rad}} + \dot{q}_{\text{acc}} + \dot{q}_{\text{ind}} + \dot{q}_{\text{melt}} + \dot{q}_{\text{crucible}} + \dot{q}_{\text{other}}, \]

where the subscript \( \text{i} \) indicates melt, crystal, crucible, and other elements of the furnace; \( \kappa \) and \( C_p \) represent the thermal diffusivity and specific heat of material, respectively; \( q_{\text{ed},i} \) is the heat source of induction heating that only has a value in which \( q_{\text{ed},i} \) is calculated by the well-established view factor method [21]. Internal radiation is treated by an artificially enhanced thermal conductivity [19], setting to a value of 17.5 W/m K [8]. The time-dependent terms eliminate during a pseudo-steady-state modeling.

The induction heating source is achieved through averaging the energy dissipation rate over one period in the crucible,

\[ q_{\text{ed},i} = \frac{c_d}{t_e} \int \left[ \frac{1}{2} \rho \mathbf{u}^2 \right] \mathbf{u} \cdot \mathbf{b} \, dt = \frac{\sigma_e \alpha_0^2}{2 t_e} (C^2 + S^2), \]

where \( \sigma_e \) is the electrical conductivity defined as the ratio of the current density to the electric field strength, and \( \omega \) is the frequency of the driving in the coil. The energy dissipation rate, \( P \), in the cylindrical coordinates due to induction heating can be calculated via

\[ P(r,z,t) = \frac{\sigma_e \alpha_0^2}{t_e^2} (C^2 + S^2 - C S \sin 2\omega t), \]

where \( C \) and \( S \) are the in-phase and out-of-phase component of the magnetic stream function, which satisfy the following equations,

\[ \frac{\partial}{\partial t} \left( \frac{1}{C} \frac{\partial C}{\partial t} \right) + \frac{\partial}{\partial z} \left( \frac{1}{C} \frac{\partial C}{\partial z} \right) = \left\{ \begin{array}{ll} -\mu_{\text{coil}} & \text{(in the coil)} \\ \mu_{\text{con}} & \text{(in the conductor)} \\ 0 & \text{(elsewhere)} \end{array} \right., \]

\[ \frac{\partial}{\partial t} \left( \frac{1}{S} \frac{\partial S}{\partial t} \right) + \frac{\partial}{\partial z} \left( \frac{1}{S} \frac{\partial S}{\partial z} \right) = \left\{ \begin{array}{ll} 0 & \text{(in the coil)} \\ \mu_{\text{coil}} \frac{\partial \theta}{\partial t} & \text{(in the conductor)} \\ 0 & \text{(elsewhere)} \end{array} \right.. \]

Fig. 1. A schematic diagram of a Cz crystal growth apparatus for sapphire crystal growth.
The stress–strain relationship of the crystal is taken as
\[ \sigma_{ij} = C_{ijkl} \epsilon_{kl} - \alpha(T - T_0) \delta_{ij}, \]
where \( \sigma_{ij} \) and \( \epsilon_{ij} \) are the stress tensor, strain tensor, and Kronecker delta tensor, respectively. \( \alpha \) is the thermal expansion coefficient, and \( C_{ijkl} \) is the elastic constant tensor. \( C_{ijkl} \) takes various forms depending on crystal structure and growth direction. The preferred growth direction of sapphire crystal for LED substrate application is the c-axis, (0001). Sapphire belongs to the hexagonal system and rhombohedra single crystal, and the elastic constant matrix is given as follows,
\[
C_{ij} = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\
C_{13} & C_{13} & C_{12} & 0 & 0 & 0 \\
C_{33} & C_{33} & C_{33} & C_{44} & 0 & 0 \\
Sym. & C_{44} & C_{44} & C_{66} & 0 & 0 \\
C_{66} & \frac{1}{2}C_{11} - C_{12}, & C_{66} & \frac{1}{2}C_{11} - C_{12}, & C_{66} & \frac{1}{2}C_{11} - C_{12},
\end{bmatrix}
\]
where the elastic constants, \( C_{11} = 497 \) GPa, \( C_{12} = 163 \) GPa, \( C_{13} = 116 \) GPa, \( C_{33} = 501 \) GPa, and \( C_{44} = 147 \) GPa [22]. It is reported that sapphire has a softening point of about 2073 K, which makes the temperature dependences of the elastic constants nontrivial for the analysis of thermal stress during growth. However, due to the unavailable data of the relationships, the fixed values of elastic constants are applied in the current stage of our study for a qualitative analysis. The elastic constants in Eq. (9a) are transformed to the conical coordinate system by the standard transformation for the—order tensor [23],
\[
C'_{ijkl} = a_{ii} C_{ijkl} a_{jj} a_{kk} C_{klrr},
\]
where \( a_{ii} \) is the vector transformation for the direction cosines between the rectangular coordinate system and the conical coordinate system. In order to make a consistency of the axisymmetric assumption displacement in the circular direction and axial directions, respectively. It is noted that based on the axisymmetric assumption displacement in the circular direction is forbidden.

After the normal and shear stresses are obtained, there are two theories regarding the analysis of the crystal cracking or dislocation generation. The first is the Maximum Principle Stress Theory, according to which failure will occur when the maximum principal stress in a system reaches the value of the maximum stress at elastic limit in simple tension. The second is the von Mises Stress (Distortion Energy Theory), which proposes that the total strain energy can be separated into two components: the volumetric (hydrostatic) strain energy and the shape (distortion or shear) strain energy. It is proposed that yield occurs when the distortion component exceeds that at the yield point for a simple tensile test. The von Mises stress is always a smaller value than maximum principle stress by definition, but it is aligned in the direction that has to support the maximum shear load. Since crystal cracking and dislocation are mostly caused by shear, von Mises stress is more appropriate for the analysis. The popular theory is to compare the critical resolved shear stress (CRSS) to the von Mises stress, and dislocation generation is presumed to occur in the regions where the excessive stress exists. The von Mises stress is calculated by
\[
\sigma_{	ext{von}} = \sqrt{(\sigma_{rr} - \sigma_{zz})^2 + (\sigma_{\phi r} - \sigma_{rr})^2 + (\sigma_{\phi z} - \sigma_{zz})^2 + 6\sigma_{zz}^2}.
\]

2.3. Boundary conditions

The following boundary conditions are applied to solve the above governing equations. The first is the general axisymmetric condition, which requires that the radial gradients along the centerline of the furnace of all the variables are zero. To calculate the magnetic field, the simulation domain should be large enough to set the boundaries of the magnetic components as zero. The thermal condition on the crystal/melt interface is derived through the total heat flux balance as follows:
\[
-\mathbf{n}_k \cdot \nabla T = -\mathbf{q}_c^\theta \mathbf{n} + \mathbf{n}_k \cdot \mathbf{q}^\theta_{c | \nabla |}. \left| \mathbf{n} \right| = \rho_s \mathbf{H} |\mathbf{u}_{\text{int}}| \mathbf{n} | | \mathbf{n},
\]
where \( \mathbf{n} \) is the unit vector of normal direction at the interface to the melt, \( k_s \) and \( \rho_s \) are the thermal conductivity and density of the crystal respectively, \( \mathbf{H} \) is the latent heat release due to solidification, and \( \mathbf{q}_c^\theta \) is the radiative heat loss across the melt/solid interface. \( \mathbf{u}_{\text{int}} \) is the interface velocity. In numerical simulation, we calculated the solidification rate at the interface and assumed that the triple point, e.g., contact point between meniscus and solidification interface, is fixed. The moving rate of the solidification interface at this point will be the pull rate. At the surface of the furnace elements where no phase-change occur, the heat balance equation becomes
\[
-\mathbf{n}_k \cdot \nabla T |_{s} = -\mathbf{q}_c^\theta + \mathbf{n}_k k_s \mathbf{e}_s \cdot \mathbf{N} |_{s} = 0,
\]
where \( \mathbf{n}_k \) is the unit vector of normal direction at the surface pointing to the environment gas, \( \mathbf{q}_c^\theta \) is the radiative heat loss across the surface of the elements, and the subscript, es, represents the fluid environment surrounding the surface. The temperatures on the furnace chamber wall and on the coil are close to room temperature due to the efficient cooling by water.

The velocity boundary conditions on all the interfaces of the furnace elements and the atmosphere gas are set to non-slip. Since the growing crystal rotates steadily during the growth, the velocity on the S/L interface is given as \( \mathbf{u}_w = \omega \mathbf{r} \), where \( \omega \) is the crystal rotation rate, and \( \mathbf{r} \) is the crystal radial position. On the free surface, the Marangoni boundary conditions are applied for the tangential stress balance,
\[
\tau_s = \frac{\partial}{\partial t} \nabla T |_{s}.
\]
where \( \partial / \partial t \) is the surface-tension–temperature coefficient, and \( s \) denotes the value of the variable at the free surface.

To calculate the thermal stress, the solid/liquid (S/L) interface and crystal surface are considered as no traction boundaries, i.e.,
\( \sigma \cdot n = 0 \). Axisymmetric boundary conditions, \( v = 0 \) and \( \partial u/\partial n = 0 \) (\( u \) and \( v \) are the displacements), are applied on the axis. The pulling of the seed rod also causes traction at the top of the crystal, but in the current study such an effect is ignored.

3. Results and discussion

The governing equations with their associated boundary conditions are mainly solved using the in-house built code, MAS-TRAPP [25], after combing with a subroutine for thermal stress calculation. The thermo-physical properties of sapphire are given in reference [20]. A reference case is chosen for a comparative analysis, whose parameters and growth conditions are given as the following. Thermal conductivity of side insulation and top insulation are 2.0 W/m K, the distance of the coil center to the furnace bottom is 250 mm, the crystal rotation rate is 2.5 rpm, the crystal radius is 55 mm, and the crystal length, i.e., the distance from the free surface to the seed rod, is 90 mm. The pulling rate is set as 2 mm/h, and the growth pressure is standard. During simulation, the heating power is adjusted to match the melting condition. The heating power is adjusted to match the melting point at the triple point. Simulation results of the reference case are presented in Fig. 2.

Fig. 2a shows magnetic field in the growth furnace. The in-phase potential has the largest value at the center of the RF coil, while the out-of-phase potential reaches its maximum on the crucible surface due to the penetration depth of the magnetic vector on the metal of the iridium. Fig. 2b presents temperature distribution in the growth furnace, the von Mises stress in the growing crystal, and stream function in the melt. The highest temperature region is around the center of the crucible sidewall, at which the maximum induction-heating resource locates. The S/L interface is convex into the melt under the current furnace design and growth parameters. The melt convection is represented by stream function, and a main vortex is observed, which is clockwise and initialized by the hot sidewall of the crucible. There is a weak counter-clockwise vortex driven by the forced convection of the crystal rotation under crystal, which can be observed from the distortion of the streamline. It is noted here that the Marangoni convection close to the free surface of the melt is driven from the hot region to the cold region, i.e., from the crucible wall to the centerline of the furnace along the free surface, due to the negative surface tension–temperature coefficient of sapphire. Therefore, the Marangoni flow has the same direction as the buoyancy flow, and the flow roll could not be observed separately. The isothermal lines in the melt are distorted by the melt convection. The von Mises stress distribution indicates that the highest thermal stress regions are close to the triple point, the seed and the interface regions. The convexity of the interface is denoted by the distance of the free surface to the lowest or highest point of the interface. The maximum von Mises stress and the convexity of the interface for the reference case are 27.0 MPa and 0.013 mm, respectively.

The insulation of the furnace for sapphire single crystal growth is double-layered due to the high melting point of this material. The ability of the insulation plays a significant role on the design of an appropriate hot zone in the furnace. The effect of thermal conductivity of the insulation on the S/L interface convexity and on the local maximum von Mises stress is presented in Fig. 3. It can be seen that as the heat insulating ability of the top insulation, \( k_{ts} \), becomes better, i.e., the thermal conductivity becomes smaller, the convexity of the interface decreases, and the maximum von Mises stress reduces significantly. A better top insulation means more heat will lose from the side of the furnace, and the heat flux in the crystal will be more vertical to the axial direction of the crystal. The normals of the crystal interface are parallel to the heat flux vector. Thus, the increase of the top insulation condition is helpful to achieve flat interface. The side insulation, \( k_{ss} \), has an opposite effect, i.e., the increase of the insulation ability leads to a more convex interface shape and a larger maximum von Mises stress. The reason is exactly the same as that for the explanation of the effect of the top insulation. A worse side insulation means more heat should lose from the side of the furnace. Therefore, a flatter interface can be achieved, and a less von Mises stress distribution will be induced. A general conclusion could be made that to achieve a flat interface heat loss from the side of the furnace should be increased, and/or heat loss from the top of the furnace, however, should be minimized. It is noted here that the conclusion is based on a convex interface shape. If the initial interface is concave, the conclusion will be reversed.

Fig. 4 gives the effect of the coil position, which is denoted by the distance from the center of the coil to the bottom of the furnace, and is 250 mm for the reference case. Fig. 4a shows the simulation results of the case with a moved-down RF coil, about 5 mm lower than the reference case. Comparing to the reference case, the highest temperature region moves down to the lower part of the crucible, which causes a dramatically variation of the flow pattern in the melt, temperature distribution in the furnace, the stress distribution in the crystal, and the convexity of the interface. From Fig. 4b one can see that as the coil position increases from 240 mm to 260 mm, the maximum von Mises stress reduces from 46 MPa to 17 MPa, however, the convexity of the interface increases from 8 mm to 16 mm. The different trends of the stress and convexity curves seem uncover a contravention of the general conclusion, i.e., a flatter interface, a less stress level.
However, it can be explained that the lower RF coil position reduces temperature at the top part of the crucible, which causes a cooler gas environment around the crystal. Thus, the temperature difference in the crystal goes up, and the maximum von Mises stress increases (see Fig. 4c). One can also see from Figs. 2b and 4a that the location with the highest stress level moves from the triple point up to the shoulder of the crystal. Since the temperature at the bottom part of the crucible goes up, more heat will go through the crystal interface, which accounts for the higher stress level around the interface. The increased heat flux through the interface has axial and radial components. The axial component may be more important than the radial one, so the interface becomes flatter. In a summary, the RF coil can slightly move downwards to achieve a flatter interface and a less stress level around the interface region, although the maximum von Mises stress in the crystal will rise up.

Fig. 3. (a) The effect of thermal conductivity of the insulation on the S/L interface convexity and (b) the effect of thermal conductivity of the insulation on the maximum von Mises stress. $k_t$ is the top insulation and $k_s$ is the side insulation.

Fig. 4. (a) The effect of the coil position (about 5 mm lower than the reference case) on the temperature distribution, melt convection, and von Mises stress distribution, (b) the effect of the coil position on the S/L interface convexity and the maximum von Mises stress, and (c) a comparison of axial temperature profiles along the axis.
Fig. 5a and b presents the effect of the crystal length and radius on the temperature distribution, melt convection, and von Mises stress distribution. The different lengths of the crystal can be used to approximately denote the different growth stages. It can be seen that as the crystal grow longer, melt convection becomes weaker mainly due to the reduction of the melt height. Comparing to the reference in Fig. 2b, the interface becomes flatter due to the decrease of the temperature gradients around the interface. In other words, the interface moves to an ambience with more uniform temperature distribution at the lower part of the crucible, and turns into a flatter shape. However, from Fig. 5c one can find that the maximum von Mises goes up significantly as crystal grow longer. From Fig. 5a, the maximum stress region is observed around the middle part of the crystal close to the heater shield. According to our former research in laser oxide crystal, the effect of the heater shield accounts for such high thermal stress levels [26,27]. From Fig. 5b, it can be found that as the crystal radius decreases, the temperature distribution in the crystal becomes more uniform, which results in the decrease of the maximum von Mises stress and the reduction of the interface convexity (see Fig. 5d). It is the reason why small high-quality crystals are easier to grow than large crystals. Conclusively, the predicted interface is largely convex into the melt when the crystal is short, and it becomes flatter as the growth proceeds. The maximum von Mises stress increases as the crystal grows longer. According to the analysis in Fig. 4b, during the growth the coil can slightly move up to achieve a constant convexity of the interface and to reduce the maximum stress level. Thus, to keep a stable growth process, the RF coil can be controlled to adjust the change of the S/L interface shape caused by the length change of the crystal.

Fig. 6 illustrates the effects of crystal rotation rate on the growth process. The effect of an intermediate crystal rotation (8 rpm) on the temperature distribution, melt convection, and von Mises stress distribution is given in Fig. 6a. Comparing to the reference case, the interface is less convex, and a strong counter-clockwise vortex driven by the crystal rotation is observed. A weak vortex around the intersection of the free surface and the crucible is also predicted. As the crystal rotation further increases, the interface becomes flat, and then concave into the crystal as Fig. 6b shows. The fast crystal rotation (18 rpm) results in much stronger forced convection, which totally suppresses the natural convection around the interface region. During simulation, a further increase of the rotation rate will make the front-tracking technique fail due to the highly distorted grids around the largely concave interface due to the enhancement of the forced convection. The effect of the crystal rotation rate on the interface convexity and the maximum von Mises stress is presented in Fig. 6c. The negative convexity means the concave interface shape. The flat interface is achieved when the rotation rate is about 12 rpm. A rotation rate larger than the value leads to the concave interface. The maximum von Mises stress reaches the minimum when the flat interface is obtained, and goes up fast as the convexity/concavity of the interface increases. The concavity has a more obvious effect on the maximum stress than the convexity does. Thus, a lower crystal rotation rate is better for the reduction of the von Mises stress; however, it is prone to form composition-related crystal defects [10].
4. Conclusions

In this paper, numerical simulation is conducted to study the temperature distribution, melt flow, S/L interface and von Mises stress distribution during a Cz-growth of sapphire single crystal. The effects of insulation condition, crystal size, RF coil design and crystal rotation rate are discussed. Based on the discussion, the following conclusions could be obtained: (1) To achieve a flat interface heat loss from the side of the furnace should be increased (the reduction of the insulation ability), and/or heat loss from the top of the furnace should be minimized (the increase of the insulation ability). The stress level at the interface region in the growing crystal can be minimized with a flat interface. (2) The RF coil can slightly move down to achieve a flatter interface and a less stress level around the interface, although the maximum von Mises stress in the crystal goes up. (3) The predicted interface is largely convex into the melt when the crystal is short. It becomes flatter as the crystal grows longer. The region with the largest stress is located at the middle part of the crystal affected by the heater shield. High-quality small crystals are much easier to grow, since a flatter interface, around which stress level is low, is more convenient to obtain during small crystal growth. (4) As crystal rotation rate changes from 2.5 rpm to 18 rpm, the interface shape transforms from convexity to concavity with a transition, i.e., a flat interface, at a crystal rotation rate of 12 rpm. When the interface is flat, the maximum von Mises stress reaches the minimum value. The above conclusions provide a basis for the improvement of growth conditions to control interface shape and to reduce thermal stress during the crystal growth.

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