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Effect of heating conditions on flow patterns during the seeding stage of Kyropoulos sapphire crystal growth

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ABSTRACT

We apply numerical simulation to understand the effect of heating conditions on melt convection in an industrial Ky furnace. The direct numerical simulation (DNS) approach was used to investigate the features of melt flow during the seeding stage. Two different cases of Kyropoulos furnace hot zone design were studied numerically, and results were compared with experimental data to understand the effect of modifications on melt convection.

1. Introduction

Lately, there has been much interest in growing large size sapphire crystals of high quality (see Fig. 1 with crystals grown in Crystal Development Ltd.). For industrial Ky furnaces, one of challenges is to achieve a good convection structure over the melt free surface, required for optimal seeding and stable crystallization speed.

Over the melt free surface a spoke pattern is usually observed, which is a result of buoyancy and Marangoni driving forces [1]. For decreasing seeding time, the most preferred is a star-like or centered regular and stable spoke pattern configuration. For example, a centered 12-fold temperature spoke pattern was observed in a small (1.4 kg melt charge) laboratory Ky furnace [2]. The reasons of this phenomenon and mechanism of forming such temperature distribution were discussed in the paper [2]. Increase in sapphire charge weight and, therefore, crucible size, complicates the free surface pattern structure and leads to form more unstable and less regular temperature distribution. One of the way to govern the melt flow and, as result, surface patterns, is optimizing the hot zone design of a Kyropoulos furnace. According to Demina et al. [3,4], modification of the furnace heat system can essentially influence the melt flow, for example, by eliminating the remelting zones near the crucible wall and by changing temperature gradient along the crystallization front. Szmyd et al. [6] found that a temperature drop on the vertical part of the crucible wall could be one of factors to provide a spoke pattern. Using CGSim software developed in STR, we apply numerical simulation to understand the influence of hot zone modification for the industrial 65-kg Ky furnace, used in Crystal Development Ltd., on forming regular and stable free surface pattern, required for optimal crystal seeding.

2. Problem formulation

2.1. Experimental results

The industrial Ky furnace, used in Crystal Development Ltd., is schematically shown on Fig. 2. The crucible radius, r_c, is 148 mm, the height h_c is 323 mm. The total power of the heater during crystal seeding was 64.4 kW. The weight of sapphire charge in the crucible was 65 kg.

Two experiments were carried out: first in the standard furnace design ("Case 1"), and second – with a hot zone modification ("Case 2").

We have obtained photos of the melt free surface for each of two cases. Photos have been recorded by electronic camera through a tinted glass, and then digitally filtered to localize the temperature minima corresponding to the areas of a lower radiation flux. Also some data of the furnace cooling system and temperature value at the center of the crucible (measured by spectral ratio pyrometer) were recorded during crystal growth, which helps us to perform detailed verification of the computer model.

In the Ky furnace, the cooling system consists of 10 separate

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Fig. 1. Sapphire 65 and 30-kg crystals.

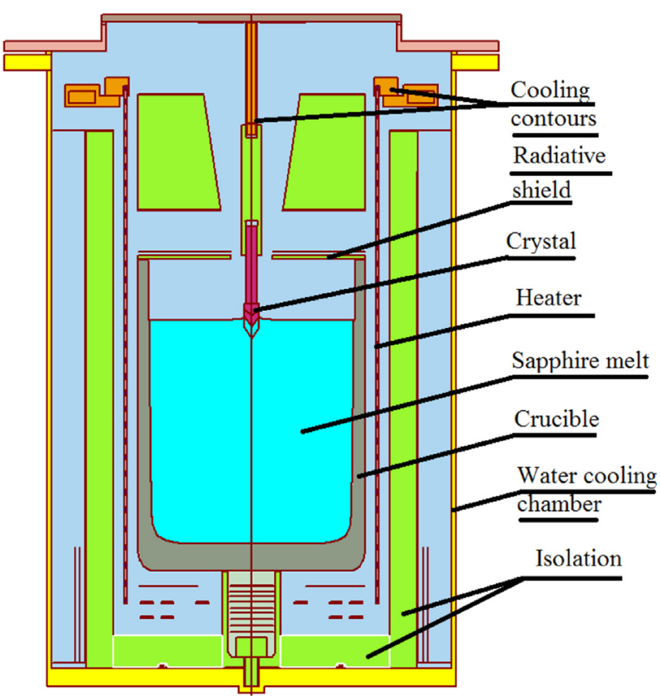

Fig. 2. A schematic view of 65-kg Ky furnace.

water flow channels for cooling the external chamber walls (see Fig. 3), pedestal, the seed holder and rods for supplying electric current. In each cooling channel, the outlet water temperature t_i and the mass flow rate G_i can be recorded during each growth run, thus consumed heat power of each cooling channel and total power $P=\sum_1^{10} c_p G_i (t_{inlet} - t_i)$ can be measured experimentally and compared to modeling results.

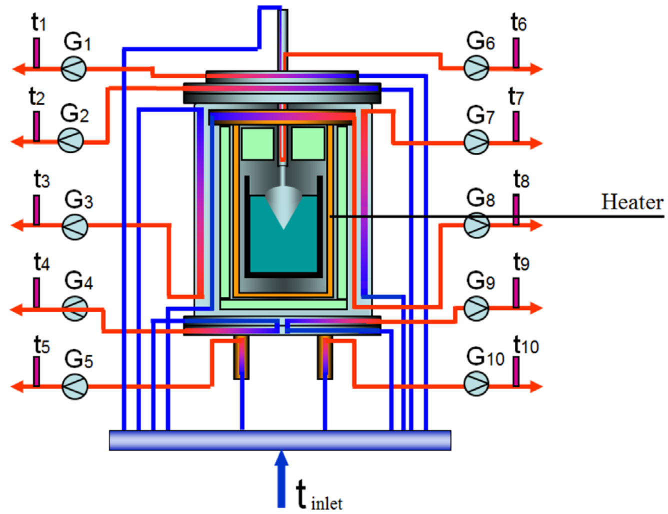

Fig. 3. A schematic view of Ky furnace cooling system.

2.2. Numerical model

Following the theory manual of CGSim software [5], the governing continuity, momentum and energy equations for the melt are written as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{u} \right) = 0, \quad (1)$$

$$\frac{\partial (\rho \vec{u})}{\partial t} + \left(\vec{u} \cdot \nabla \right) \rho \vec{u} = - \nabla p + \nabla \cdot \underline{\tau} + (\rho - \rho_0) \vec{g}, \quad (2)$$

$$\frac{\partial (\rho c_p T)}{\partial t} + \nabla \cdot \left(\rho c_p \vec{u} T \right) = \nabla \cdot \left(\lambda_{eff} \nabla T \right) - \nabla \cdot \vec{q}_{rad}, \quad (3)$$

$$\tau_{ij} = \mu_{eff} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu_{eff} \delta_{ij} \nabla \cdot \vec{u}, \quad (4)$$

Here, ρ is the density, ρ_0 is the reference density, $\vec{u}$ is the velocity, $\underline{\tau}$ is the stress tensor, $\vec{g}$ is the gravity vector, p is the pressure, $\mu_{eff} = \mu_{molecular} + \mu_{turbulent}$ is the effective dynamic viscosity (the sum of molecular and turbulent viscosities), c_p is the specific heat, T is the temperature, δ_{ij} is the Kronecker delta, p_0 is the reference pressure, $\vec{q}_{rad}(\vec{r}) = \int_0^\infty \oint_{4\pi} \vec{\Omega} I_\lambda(\vec{r}, \vec{\Omega}) d\vec{\Omega} d\lambda$ is the vector of radiative heat flux, $I_\lambda(\vec{r}, \vec{\Omega})$ is the intensity of radiation at point $\vec{r}$ in the direction $\vec{\Omega}$, λ is the wavelength of radiation. The value I_λ is found by solving the steady-state radiative transfer equation in a semi-transparent sapphire crystal (without scattering):

$$\vec{\Omega} \cdot \nabla I_\lambda + \beta_\lambda I_\lambda = \Omega_x \frac{\partial I_\lambda}{\partial x} + \Omega_y \frac{\partial I_\lambda}{\partial y} + \Omega_z \frac{\partial I_\lambda}{\partial z} + k_\lambda I_\lambda = F_\lambda, \quad (5)$$

where $F_\lambda = k_\lambda I_{b,\lambda}$, $I_{b,\lambda}(T)$ is the monochromatic black body radiation intensity and T is the medium temperature, k_λ is the absorption coefficient. The melt block is considered to be opaque with effective thermal conductivity.

2.3. Boundary conditions

On the solid wall, the velocity is set to zero.

The normal velocity component on the melt free surface is set