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Investigation of cracks formation in sapphire crystals

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Abstract. The analysis of the possible reasons of cracks formation in the sapphire crystals received by the horizontally directed crystallization method on the basis of the received results of numerical simulation of thermoelastic tension in the sapphire crystal is carried out.

1. Introduction
The big size sapphire crystals growth with improved structural characteristics became a priority of modern science and equipment. In the last decades the Czochralsky’s method, Kiroopoulos’s method, the horizontally directed crystallization (HDC) method and Stepanov’s method were applied for big size monocrystals growth. These crystals were widely used in electronic technique [1].

The sapphire crystal quality can be characterized by the orientation, density and the nature of dot defects distribution, density of single dislocations, an extension of cracks and blocks borders and their disorientation, the value of residual tension, chemical purity and impurity heterogeneity [1-3].

2. Mathematical simulation of cracks formation in sapphire crystals
There is thermoelastic tension during sapphire crystals growth in the field of temperature gradients. High level of thermoelastic tension in crystals can lead to the crack emergence in sapphire structure. In this case, it is necessary to calculate thermoelastic tension and to develop the software allowing to simulate heat exchange and tension fields at various stages of sapphire crystals growth. Mathematical simulation and calculations should be carried out for all equations which are included in the system, namely: the equations of heat conductivity and thermal elasticity.

These equations [4,5] can be written as:

\[
\begin{align*}
\mu \Delta u + (\lambda + \mu) \frac{\partial^2 \xi}{\partial x^2} &= - \frac{\partial (aT)}{\partial x} - F_x, \\
\mu \Delta v + (\lambda + \mu) \frac{\partial^2 \eta}{\partial y^2} &= - \frac{\partial (aT)}{\partial y} - F_y, \\
\mu \Delta w + (\lambda + \mu) \frac{\partial^2 \zeta}{\partial z^2} &= - \frac{\partial (aT)}{\partial z} - F_z, \\
\frac{\partial}{\partial x} (a_t \frac{\partial T}{\partial x}) + &\frac{\partial}{\partial y} (a_t \frac{\partial T}{\partial y}) + \frac{\partial}{\partial z} (a_t \frac{\partial T}{\partial z}) = 0.
\end{align*}
\]
where \( F_x, F_y, F_z \) are the components of volume sources; \( u, v, w \) are the components of displacements; \( \alpha \) is the coefficient of volume heat expansion; \( \lambda \) and \( \mu \) are the Lame coefficients; \( \Delta \) is the Laplace operator; \( i = 1,2,3 \) are the crystal, melt and crystal powder, respectively; \( a_i \) is the thermal diffusion coefficients; \( T \) is the temperature.

The boundary conditions for the system (1) are written in the form of relations as previous author’s research [6].

The simulation technique and three-dimensional numerical model are developed for calculation of temperatures, displacements, deformations and tension fields at various stages of sapphire growth by the HDC method. It allows carrying out the analysis of the temperature and thermoelastic fields changes in crystal depending on spatial and geometrical characteristics of heaters by means of computing experiment. So on the basis of the analysis, we can redistribute defects in sapphire, thereby having increased quality of the crystals.

The technique of temperatures, displacements, deformations, tensions calculations in system crystal–melt includes the following:

1. The input of basic data: density, heat conductivity and specific thermal capacity of materials, length, height and width of the crucible, Lame coefficients and some other.
2. Calculation of temperatures distribution in crystal–melt system.
3. Calculation of temperatures gradients in crystal–melt system by the method of smallest squares.
4. Displacement calculations as the first approximation in crystal–melt system.
5. Calculation of displacement gradients by the method of the smallest squares and the solution of thermoelasticity equation taking into account gradients of displacements.
6. Calculation of deformations in crystal–melt system on the basis of the received displacements.
7. Calculation of tension in crystal–melt system on the basis of the received deformations.
8. The conclusion of results.

Results of tension calculation are presented in figure 1. In figure 1 it is visible that there is compression tension along lateral faces of the crystal, and at the middle part of the crystal, it can be seen stretching tension. The size of thermoelastic tension depends on the distribution of temperatures.

![3D scalar field Levelset](image)

**Figure 1.** Results of tension calculation in sapphire in crystal–melt system at the vertical section of crystal (the scale is in Pa).

The model for calculation of temperatures, displacements, deformations and tension fields during sapphire growth allows us to apply the numerical experiments and to study the influence of input parameters on the crystals quality. This approach allows to improve the crystal growth process and to receive the crystals with reduced defects level.

The crack in sapphire structure begins to extend when the stress intensity coefficient reaches critical value for this material [1]:

\[
K_c = 3.2 \cdot 10^5 \cdot N \cdot m^{3/2},
\]  

(2)
The results of numerical simulation of thermoelastic stresses in sapphire crystals received by authors earlier were used for the analysis of the possible reasons of cracks formation in the sapphire crystals which are received by the HDC method. The model included calculation of temperatures, displacements, deformations and thermoelastic stresses of the growing sapphire crystal by the method of control volumes on the unstructured grid [6-7].

Critical value of stress intensity coefficient is defined by formula [7]:

$$ K_c = \sqrt{2E\gamma}, $$

where $E$ – Young's modulus; $\gamma$ – the specific superficial energy of sapphire.

We use the following sapphire parameters for simulation [7]: Young's modulus is $E = 460 \text{ GPa}$ and specific superficial energy of sapphires $\gamma = 1.1 \text{ J/m}^2$ when critical stress intensity coefficient is (2).

Cracks growth can lead to sapphire fragile destruction. Cracks can suddenly become unstable in sapphire structure and extend into a material with a certain speed.

Sapphire fragile destruction appears when stress intensity coefficient equals to critical value of stress intensity coefficient [1,7]:

$$ K = K_c, $$

when $K = \sigma(\pi a)^{1/2}$ is the stress intensity coefficient; $\sigma$ is the stress; $a$ is the crack length.

On the basis of stresses calculations during sapphire crystal growth by HDC method, the estimation of formed cracks length in sapphire crystals was made. Fragile destruction of sapphire can appear when the crack in material reaches some critical length at the fixed stress, i.e. for the fixed thermoelastic stress $1.99 \text{ MPa}$ the critical crack length will make $0.0082 \text{ m}$.

3. The investigation results

The initial crack emergence is a consequence of high value of internal thermoelastic stresses in sapphire crystal. Further development of crack happens gradually in the sapphire growth process, and it can be connected with a relaxation of thermoelastic stresses. The suggested model adequately describes the influence of thermoelastic stresses on cracks formation in sapphire and can be used for sapphire crystals growth technological process improvement. On the basis of the model the optimum modes of sapphire, crystals growth are chosen. It allows excluding cracking during sapphire growth.

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