Journal of Physics: Conference Series

PAPER • OPEN ACCESS

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To cite this article: Y V Klunnikova *et al* 2019 *J. Phys.: Conf. Ser.* **1236** 012030

IOP Conf. Series: Journal of Physics: Conf. Series **1236** (2019) 012030 doi:10.1088/1742-6596/1236/1/012030

Computational approach to the simulation of sapphire crystals growth by horizontal directed crystallization method

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Abstract. In this article we present an integrated approach to sapphire crystals growth simulation. Thermally induced stresses in sapphire crystals growing by horizontal directed crystallization are simulated by finite element method. The simulation results correspond to experimental observations. The results of the investigation allow to improve the process of crystal growth to obtain high quality large sapphire crystal.

1. Introduction

Sapphire (α-Al_2O_3) is one of the promising materials nowadays. Due to the unique combination of physicochemical and optical properties (high melting temperature, low friction coefficient, high hardness, chemical inertness, optical transparency in a wide range of wavelengths, high strength and thermal conductivity, radiation stability and high resistance to thermal shock), sapphire is an important material, which is widely used in micro- and nanoelectronics [1-2].

In recent decades, horizontal directed crystallization (HDC), Czochralski, Kyropulos and Stepanov methods are used for obtaining large-size sapphire monocrystals for electronic engineering. The HDC is one of the most widespread method for sapphire crystals growth from melt [1-6]. During crystallization, the shape of the crystal has a significant effect on the sapphire crystal growth and defect formation. The study of the structure formation process, impurity distribution, and the nature of the defects in the crystal during growth are particularly interesting because sapphire crystals obtained by the HDC method have a characteristic configuration at the initial and subsequent stages of growth.

The vacuum heating unit for sapphire crystals growth by HDC method consists of a container with the raw material, molybdenum or tungsten heat shields and graphite insulation [7]. The crystals grow at very high temperatures (approximately 2050 °C). The interaction of melt evaporation products with a vacuum heating unit and heat shields, as well as with a heater, can have a negative effect on the crystallization process. Requirements for the sapphire quality depend on their application field. However, thermoelastic stresses usually reduce the strength and decrease durability of sapphire elements. The stresses in sapphire crystals could lead to cracks. Therefore, it is important to decrease the thermal stresses to obtain a crystal with good mechanical and optical characteristics.

In our early research we investigated the sapphire crystal shape factor influence on its growth and defects formation such as bubbles during sapphire growth [8, 9]. In this paper we present the stresses formation during sapphire crystals growth. Also we experimentally evaluated and calculated the

distribution of the thermal stresses during the growth of sapphire crystals by horizontal directed crystallization method.

Computational models for the stresses simulation that focus on predicting sapphire quality are under investigation for several years [10-12]. Only few theoretical works describe the stresses in sapphire crystals [14-21]. The aim of this contribution is the incorporation of the findings into overall modelling approach for computational investigation of possible defects formation during sapphire crystals growth.

Nowadays, quite detailed three-dimensional computations for stresses prediction in sapphire crystals are available. However, the open question remains on modelling the cone part of the crystal received by horizontal directed crystallization method.

2. Investigation methods

Temperature gradients cause thermo-elastic stresses during sapphire growth. In order to properly predict defects it is necessary to calculate the temperature distribution in sapphire crystals growth chamber by the horizontal directed crystallization method. Finding the temperature distribution in crystal-melt system requires solving heat conductivity equations [22-24].

As long as the container moves quite slowly, we can conclude that sapphire crystal growth is in quasi steady state and the temperature distribution can be found by the following equation [6, 22-24]:

$$div(\lambda_i(T)gradT_i(x,y,z)) = 0, \tag{1}$$

where λ_i is the thermal conductivity coefficient which depends on the temperature ($i = 1,2$ refer to the crystal, melt respectively); T_i is the temperature in crystal, melt.

The boundary conditions for equation (1), that reflect continuity of thermal fields and fluxes on boundaries of crystal-melt environments section, can be found from the following equations:

$$\lambda_1(T)\frac{\partial T_1(x_C,y,z)}{\partial x} = \lambda_2(T)\frac{\partial T_2(x_C,y,z)}{\partial x}, \tag{2}$$

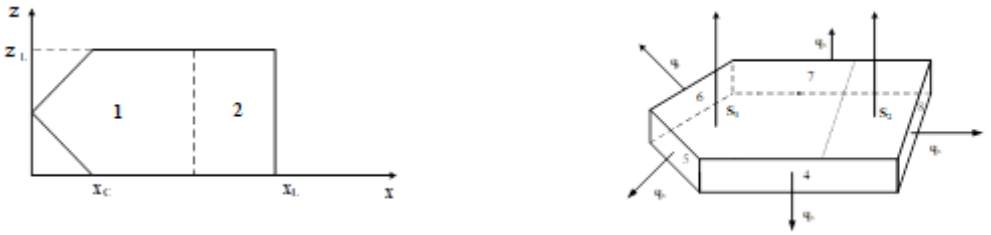
$$q_{s_1} = q_{s_2} = \sigma\beta(T^4 - T_{hot}^4), \tag{3}$$

$$q_s = 0, \tag{4}$$

where σ is the Stefan-Boltzmann constant; β is the radiation coefficient; T_{hot} is the heat temperature distribution function, q is the heat flux.

The result of temperature calculation (figure 2(a)) is used for simulation defects distribution such as stresses and cracks at various stages of sapphire crystals growth. We used the finite volume method for temperature calculation.

Simulating the stresses during sapphire crystals growth was carried out using finite element method [22-26]. We used the linear tetrahedral elements. The code was developed in the high level programming language Python.



(a) (b)

Figure 1. Schemes for calculation of HDC process: (a) 1 – crystal; 2 – melt; (b) 4, 5, 6, 7, 8 – side surfaces of crystal; S1, S2 – upper and lower boundaries.

The element stiffness matrix is given by

$$\{\mathrm{k}\} = V[B]^T[D][B], \tag{5}$$

where V is the volume of the tetrahedral element.

Once the global stiffness matrix K is obtained we have the following structure equation:

$$[\mathrm{K}]\{\mathrm{U}\} = \{F\}, \tag{6}$$

where U is the global nodal displacement vector and F is the global nodal force vector.

The strain matrix can be find as

$$\boldsymbol{\varepsilon} = \mathbf{Bu}, \tag{7}$$

where $\mathbf{B}$ is the strain-displacement matrix, $\mathbf{u}$ is the element displacement vector ($\mathbf{u} = \{u; v; w\}$).

The stress-strain $\boldsymbol{\varepsilon}$ relation can be described as

$$\boldsymbol{\sigma} = \mathbf{D}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{\mathbf{th}}), \tag{8}$$

where $\mathbf{D}$ is the elasticity material matrix, $\boldsymbol{\varepsilon}_{\mathbf{th}}$ is the initial strains induced by thermal expansion.

The boundary conditions for equations (6)-(8) for all boundaries except top one (figure 1(b)) is $u = v = w = 0$. The top boundary condition is $\sigma_{yy} = \sigma_{yx} = \sigma_{yz} = 0$.

The finite element method [24-26] for displacements, strains and stresses calculation in sapphire crystals is formulated as follows:

1. The displacement components u, v and w over a typical finite element are represented approximately as a linear combination of their values and values of their derivatives at a prescribed number of nodal points.
2. The element stiffness matrixes are calculating using the principle of minimum potential energy.
3. A global stiffness matrix K is obtained by connecting all of the elements together and applying appropriate boundary conditions. This gives us the equilibrium equations governing the connected assembly of elements.
4. The equilibrium equations are solved and stresses in a typical element are evaluated by direct substitution of local displacement field into an appropriate constitutive equation [27].

3. Investigation methods

Results of displacements calculation are presented in figure 2 which influence the stresses values. The thermoelastic tension depends on distribution of temperatures.

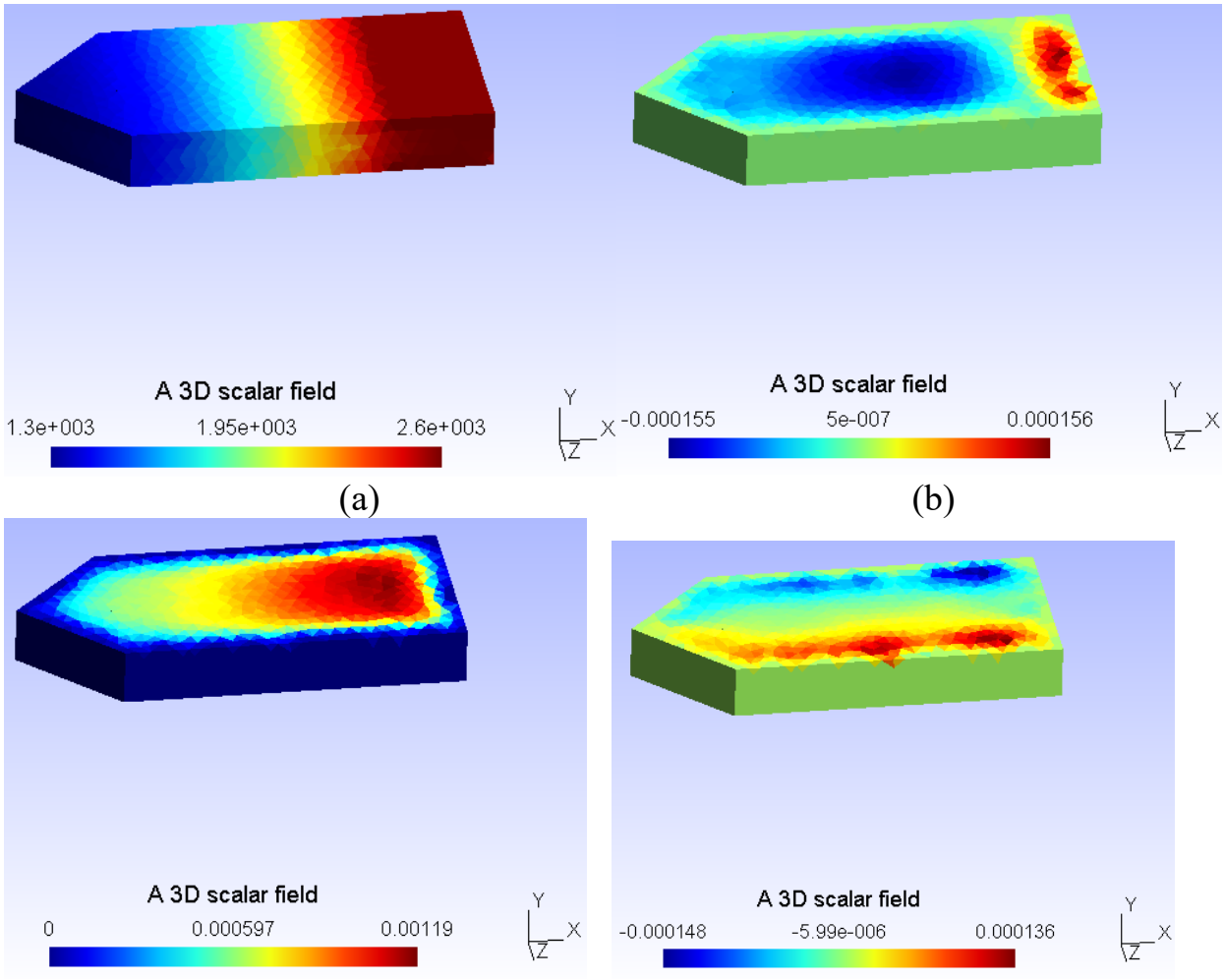


Figure 2. (a) Results of temperature calculation (in K); (b) results of u calculation (in m); (c) results of v calculation (in m); (d) results of w calculation (in m) in crystal-liquid system.

The results of numerical simulation of thermoelastic stresses in sapphire crystals are used for the analysis of the possible reasons of cracks formation in the sapphire crystals which are received by the HDC method. The model includes calculation of temperatures, displacements, deformations and thermoelastic stresses of the growing sapphire crystal by the finite element method on the unstructured grid.

The experimental study of stresses in sapphire crystals is focused on a polarization-based method that was found to be the most applicable as sapphire defect mapping tool. The experiments confirmed the results of simulation.

Therefore, the presence of temperature gradients leads to thermal stress in the crystal. If the thermal stresses exceed the material ultimate strength, the conditions for the structure defects formation will be created in the crystal volume.

In order to avoid defects formation, it is necessary to control the crystal growth process. The lower thermal stresses during sapphire crystals growth allows us to decrease sizes and density of defects in a

crystal. The presence of unevenly distributed thermal stresses exceeding the critical strength limit of the material causes intense plastic flows in the growing crystal, which can lead to an intense formation of dislocations [6].

4. The investigation results

Temperature gradients cause thermal stress in the crystal. If thermal stresses exceed the material ultimate strength, the conditions for the structure defects formation occur in the crystal.

We present a computational model for the analysis of sapphire crystals stresses formation. We also describe the fundamentals of the underlying numerical methods for the study thermoelastic stresses in sapphire crystals.

The model for calculation of temperatures, displacements, deformations and tension fields during sapphire growth allows us to make 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 suggested model describes adequately the influence of temperatures on stresses formation in sapphire. On the basis of the model we choose the optimum modes of sapphire crystals growth. It allows to eliminate defects formation during sapphire growth.

Acknowledgments

This work in Southern Federal University and Leibniz University of Hanover was supported by the Ministry of Science and Education of the Russian Federation and the German Academic Exchange Service (DAAD) within the framework of the joint program “Mikhail Lomonosov”.

This work in the Peter the Great St. Petersburg State Polytechnic University was supported by the Ministry of Science and Education of the Russian Federation, project no. 3.1150.2017/4.6.

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