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## MATHEMATICAL MODELS OF THERMAL PROCESSES IN THE MULTI-ZONE THERMAL INSTALLATIONS FOR GROWING CRYSTALS

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#### Introduction

The needs of practice constantly stimulate the need to increase the geometric dimensions of the grown crystals and therefore toughening of requirements to their quality. This is especially true for non-linear optical crystals, which must operate at high laser intensities, and therefore have a low optical loss and high optical damage threshold [1]. Experimental studies show that the most effective non-linear optical materials for the conversion of infrared radiation in the terahertz are single crystals of compound ZnGeP2. At present developed the technology of growing single crystals ZnGeP2 of required quality by the Bridgman method with a diameter of 30 mm and a length of 200 mm in the multi-zone thermal installations (MTI). However, to create terahertz radiation converters needed samples with a diameter of 50 mm. As a rule, a simple increase in the sizes of the working volume MTI and growth containers (GC) does not allow obtaining a single crystal of a larger nominal value, and leads to a decline in the quality and the deterioration of the physical characteristics of the sample. This is caused by many of physical and technical problems associated primarily with the problem of providing the assigned temperature conditions with the required accuracy. Because of the complexity of heat transfer processes occurring in the conversion of the melt into the crystal, the lack of technical measuring means of the temperature field near the crystallization front, predicting behavior of temperature field without the use of computer models is not possible.

Therefore one of the urgent problems arising in the development and improvement of MTI is the creation of mathematical model that allows for real-time to predict with acceptable accuracy during the process of crystal growth in varying thermal conditions.

#### **Constructive form MTI**

The main element of MTI is the thermal module. The most wide practical application found by thermal modules cylindrical geometry. Assembling consistently put on each other modules enclosed in a single sheath surrounding air space with the ambient temperature, forming MTI (Fig. 1.). For growing crystals in the center of MTI provided a cylindrical cavity, called the workspace. In this cavity on a stand is placed GC with the working substance from which the crystal is grown. The temperature field of installation formed by means of electric heaters of thermal modules so that in the upper zone of the working substance in the molten state, and in the lower zone in the solid state. In the middle zone there is a transformation of the working substance from the initial state to the melt while GC moving up and crystal formation when GC moving down. To obtaining crystals with high optical qualities necessary that the crystallization temperature was situated in the middle zone and was maintained with a predetermined accuracy, despite the movement of the RK and the processes of conversion of the working substance in the various states, accompanied by the absorption of the heat (with melt) or release of heat (during crystallization). To increasing the accuracy of formation of the temperature field in the gradient zone of thermal modules manufactured with two heaters located in the areas with different thermal insulation properties [2]. The inner region is executed with high thermal conductivity of the insulator to achieve uniformity of thermal field in the crystal growth and of expeditious transfer of heat energy generated in the heaters in the work area. In the outer region using the insulator with low thermal conductivity for the creation of the base of temperature field of middle-zone and reduce heat loss to the surroundings. In addition, this arrangement significantly reduces the influence of ambient temperature change on the temperature field in the working volume MTI, and, consequently, in GC.

### Simplified mathematical model of the MTI

Models, the maximum reflecting the peculiarities of growing crystals in MTI, implemented by the finite element package COMSOL. They require a significant amount of computational resources and time-consuming for the simulation of automatic control systems. Therefore designed a simplified model MTI in the package Matlab to provide quick calculation of the temperature field of installation and GC. It allows operatively get a lot of versions of the calculations in the optimization of operating conditions MTI.

In accordance with the axial symmetry of installation, in the design scheme of vertical cut is divided into 290 cells (58 in height and radius 5) (fig.2). Each cell is exchanging thermal energy with neighboring. On the external surfaces of the installation, convective heat exchange with the environment. The exchange of thermal energy between installation and works volume attributes by using heat conduction and radiation. Equation describing heat processes in each cell of the MTI and the GC has the form:

$$(c\rho V)_{i,j}\frac{dT_{i,j}}{dt} = \sum_{s=1}^{5}Q_s, \quad i = 1,...,N; j = 1,...,5$$

Where V is the volume of the cell;  $Q_{1-4}$  is component thermal flow entering the cell from adjacent cells;  $Q_5$  – is thermal power released a heater located in the corresponding cell of the MTI. Components of heat flow into the cell from the outside, is calculated depending on its location. Power dissipated in the cell by placing of the heater, for modeling the MTI is calculated by the regulator. Calculation scheme model, implemented in the environment of Matlab, is shown in Fig.2.



Fig. 1. Fragment of the MTI, filled with the attributes associated with crystal growth process. Legend: 1) insulation material; 2) stand installation; 3) heating modules; 4) heater; 5) GC (ampoule with crucible containing the working material); 6) working material; 7) GC support

	Working volume Γ3				MTI		
E1	N,1	N,2		N,3	N,4	N,5	-
	N-1,1	N-1,2		N-1,3	N-1,4	N-1,5	
	N-2,1	N-2,2		N-2,3	N-2,4	N-2,5	
	31,1	31,2		31,3	31,4	31,5	Γ4
	30,1	30,2		30,3	30,4	30,5	
	29,1	29,2		29,3	29,4	29,5	
	5,1	5,2		5,3	5,4	5,5	-
	4,1	4,2		4,3	4,4	4,5	
	3,1	3,2		3,3	3,4	3,5	
	2,1	2,2		2,3	2,4	2,5	
	1,1	1,2		1,3	1,4	1,5	
		Ге	5]	Γ5 Γ2			-

Fig. 2. A simplified calculation scheme of MTI

When conducting computational experiments on model realized in the program package COMSOL, it is assumed that the regarding area can be quite satisfactorily approximated ~ 62000 elements, and in the simplified model - 290 elements. The calculations were performed for the levels of power heaters, accounting for 50% of the rated power and the position of the GC  $H_0 = 0.7$  m. Time calculation is 526000 s.

The calculation results in the form of the temperature distribution along the height of the working volume at r=0.008 (1), r=0.023 m (2) and MTI at r=0.066 (3), r=0.133 (4), r=0.198 (5), r=0.23 (6) m shown in Fig. 3.





The figures show that the temperature field MTI, obtained on different models quite correspond each other. However, this time the calculation of the stationary state in COMSOL is much higher than in Matlab, which confirms the efficiency and accuracy of the simplified model.

## Conclusion

1. Development of non-stationary computer model MTI on the COMSOL, allowing simulate the thermo-physical problem with the growing crystal, showed sufficient flexibility and effectiveness of our approach for the calculations of MTI with a complex geometric structure.

2. Simplified dynamic model for the calculation scheme is suitable for operational decision problems that arise both at the stage designing new structures MTI, and at the stage growing crystals.

3. To achieve high accuracy results of the calculations crucial is completeness of the registration of the real structure and the diversity of the physical properties of materials MTI, it is easier to make in COMSOL. At the same time the problem of searching of acceptable control algorithms more expedient decide on a simplified model that is implemented in an interactive environment Matlab.

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## DESIGN OF THE FEEDBACK CONTROL SYSTEM TO CONTROL THE EXTRUSION PROCESS

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### Introduction

A rapid prototyping method makes it possible to produce complicated parts based on computer 3D model. Most of the rapid prototyping methods can assemble models from a variety of widespread and special materials. The modern additive technology for most of 3D-printers requires ABS-filaments or PLA-filaments, respectively, from ABS (Acrylonitrile butadiene styrene) polymer or PLA (Polylactic acid) polymer, with a diameter of 1.75 mm or 2.85 mm, which are used as a consumable material in 3D printing technology.

Filament is obtained from plastic granules, which in case of ABS, are the products of oil and gas industry. Accordingly, the price of granules is much cheaper than the price of the finished product, even taking into account the cost of electricity consumed in transformation of the granulate in the filament.

In this article, factors affecting the diameter of plastic filaments are investigated, the problem of improving the quality of the filament plastic in the extrusion process is considered.

## Statement of the problem

A great deal of the research has been conducted at universities and research institutions to expand the applications of FDM technology and to improve the FDM process. The work has also been in progress in some organizations to develop new metallic or ceramic materials for rapid fabrication of functional components by FDM with higher mechanical properties [2, 3].

In operations of the 3D-printer, the basic parameter affecting the quality of the finished product and fidelity digital models is the diameter of