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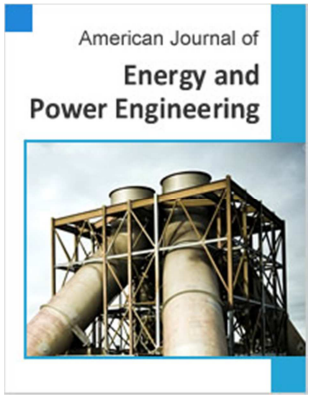

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Numerical Simulation of Heat Transfer in a Furnace Heating Unit for Horizontal Direct Crystallization of Sapphire Single-Crystal

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Abstract

Verified numerical simulation of heat transfer through the structure is an effective tool that allows to shorten development time and reduce development costs. The thesis describes numerical simulation of heat transfer in a heating unit structure for sapphire single-crystal growth. Heat transfer through radiation and conduction was simulated using commercial FEM software. As time dependent simulation requires high computing capacity, the 3D model has been simplified. The calculated temperature values are compared with the measured temperatures during the crystal growth process. This analysis is aimed at assisting in the construction design of similar heating units or in optimization of the current heating unit.

1. Introduction

Nowadays, there is a growing interest in the production of sapphire single-crystal due to its unique properties, such as high optical transparency, transmission over a broad wavelength range, etc. These properties predispose sapphire for use at high temperatures, pressures and in chemically aggressive environments. Sapphire single-crystals and related single-crystals are widely used in various areas such as medical implants, optical devices, watches, etc. They play an irreplaceable role in photonics and microelectronics. They are used for manufacturing laser components and in the defense industry as transparent armor [1] [2].

One of the methods also used for their production is horizontal direct crystallization (HDC), which provides for the growth of high quality crystals of large dimensions in the shape of a plate [3]. A heating unit of a vacuum crystallization furnace for the HDC method consists of a container filled with the raw material; a set of molybdenum or tungsten heat shields around the heaters and graphite insulation. The heating unit is

placed in a water-cooled vacuum chamber. Crystal growth occurs at very high temperatures; with the temperature of the heating unit structure components reaching approximately 2,200°C. This actually eliminates the possibility of experimental measurements in areas with the highest temperature. In addition, high temperature significantly limits the application of affordable refractory materials. Therefore, the production of heating unit components is demanding and the components are costly.

Another task that needs to be addressed is the management of electricity consumption. Crystallization takes place in an electric resistance furnace. Achieving the required melting temperature requires a direct current source with a power of several tens of kW. This power is then required to cool down in the vacuum chamber housing. This is an energy-intensive process. The task of optimizing heat transfer is to reduce the energy consumption in the process and thus reduce production costs, together with all the positive effects on the environment.

Due to these reasons, numerical simulation is an effective tool for an analysis of processes in a heating unit. It enables evaluating important parameters such as the temperature, heat flow, including time dependent, and in different parts of the structure. At the same time, there is no need to manufacture the necessary components or to conduct complex and expensive measurements for every alteration.

Numerical heat transfer simulation in a furnace heating unit for HDC has its particularities. Firstly, it is the material used. The physical parameters of refractory materials used at such high temperatures are not commonly available or are even completely unavailable [4]. They can be acquired through demanding experimental measurements or they can be determined indirectly. Furthermore, such verification of simulation results is demanding with respect to high temperatures and vacuum. These problems are most obvious when simulating the physical processes in the melting container in which both the raw material's solid and liquid phases and the resulting single-crystal are present.

The physical processes in a melting container are rather well-controlled in the simulation of crystallization of other single-crystal growth methods [5-10]. The application of this knowledge for the HDC method simulation is a separate topic as well as research task. Several workplaces around the world have been dealing with this task [11-17]. What these tasks have in common is a detailed simulation of the processes in the crystallization container. A heating unit is usually replaced with a simple casing with basic heat transfer parameters. These simulations, however, do not provide enough information required for a detailed design of a heating unit, which was one of the impulses for this project. For the purposes of this project a simplification was applied by removing the crystallization container from the heating unit, whereas verification measurements were conducted under the same conditions. The simulation thus only focused on the details of the furnace design.

2. Numerical Simulation

Due to an extensive time analysis (approx. 14 hours), the heating unit model had to be simplified (Figure 1) so as to contain the least number of elements after meshing. It consists of heaters, supporting part and insulation. The shape of the heaters was modeled with a rectangular cross section.

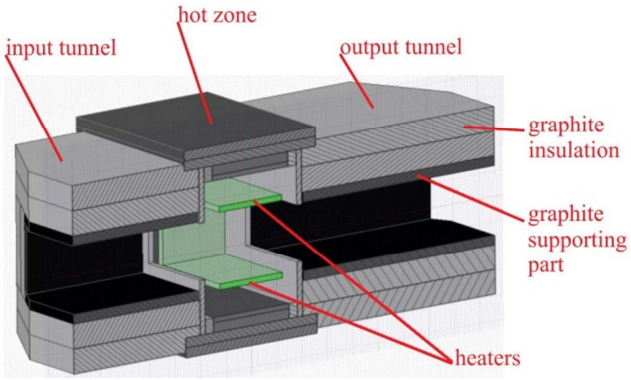

Figure 1. *Simplified heating unit model.*

The convection boundary condition was applied to the outer walls of the heating unit. The boundary condition simulates heat exchange between the heating unit and the inner wall of the vacuum chamber. Container with a charger was omitted (Figure 2). The temperature input parameter for the heaters was defined as seen in the graph (Figure 3). The temperature was obtained by real measurements. Its value is time-dependent (Figure 3) and can be divided into two phases, the start-up phase until 32,400 seconds (9 hours) and the final temperature phase until 50,000 seconds (approx. 14 hours). The temperature of the heaters is stabilized when a balance is struck between the power supplied to the heater and the power that is drawn from the surface of the heating unit. Breaks on the chart during the start-up phase are changes in the growth speed of power to the heaters. They are caused by technological process requirements. The difference in temperature between the heaters is due to structural differences and their different power, which is also a technological parameter.

The model is filled up with a combined grid structure consisting of hexahedrons and tetrahedrons. This type of grid can adapt to all of the model details. The total number of elements in the presented simulation is approximately 30,000. There is no modeled gap between individual blocks while heat transfer by conduction is considered instead of radiation. The calculation had a stable course for a total duration of approximately 5 hours. The physical properties of the materials that had to be entered were: thermal conductivity, specific heat, emissivity and density.

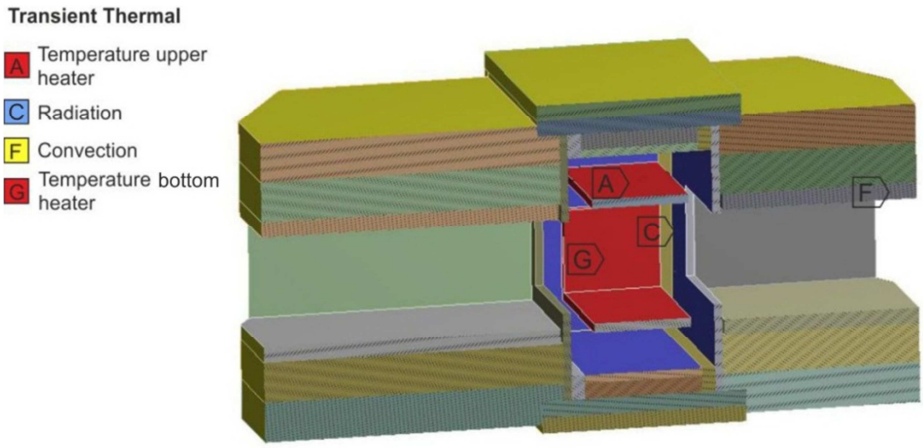

Figure 2. *Thermal simulation boundary conditions.*

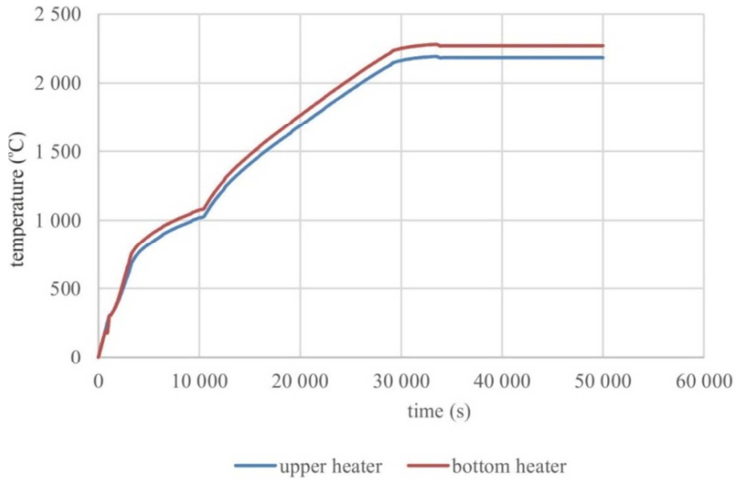

Figure 3. *Heater temperature time dependency.*

3. Results

Figure 4 shows the temperature fields in the heat unit section at individual time points. The hottest part at 50,000 seconds is the bottom heater with a temperature of 2,270°C. The coolest part is on the graphite insulation surface with a temperature of 611°C.

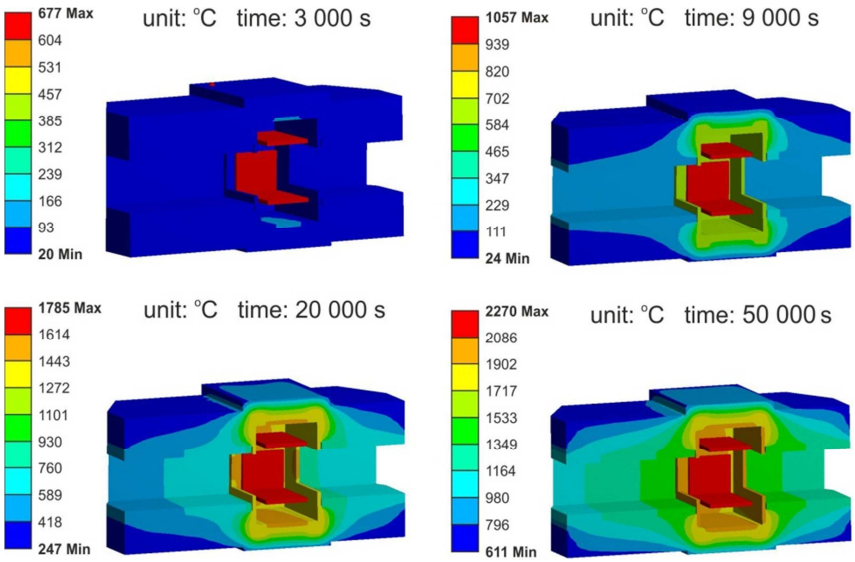

Figure 4. *Temperature fields in the section of the heating unit.*

The whole simulation had to be verified by experimental measurement. Therefore, four tungsten-rhenium type C thermocouples (Figure 5a) capable of measuring temperatures up to 2,320°C (short-term) were incorporated into the device. The thermocouples are located at the top of the exit tunnel 70 mm apart from each other (Figure 5b). Their electrical voltage is recorded over the course of the process and consequently converted into temperatures. Measurement points were defined at the same points of the simulation model to evaluate temperatures from the total time course (Figure 5c). Unlike the simulation, during the measurement, a crystallization container with raw material was inserted in the inlet tunnel of the heating unit. The graphical analysis (Figure 6) shows the approximation of simulation results to the actual measured temperature values. Between 5,000 to 20,000 seconds, the simulation temperatures are up to 200°C higher than real temperatures which can be a result of the loaded container with the raw materia, the simplified simulation model and insufficiently defined physical properties of the materials. It can also be seen that thermocouple t4 recorded considerable deviations of the measured variable which was probably caused by it being damaged.

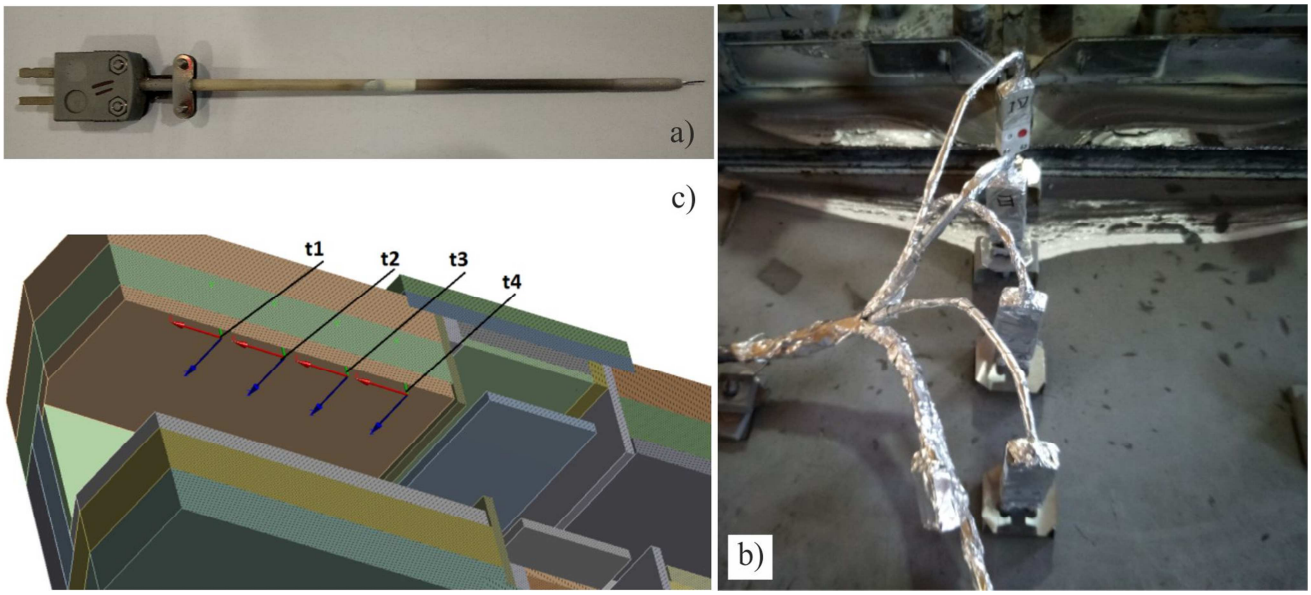

Figure 5. *a) tungsten-rhenium thermocouple type C, b) positioning of thermocouples in the heating unit, c) positioning of simulation measurement points.*

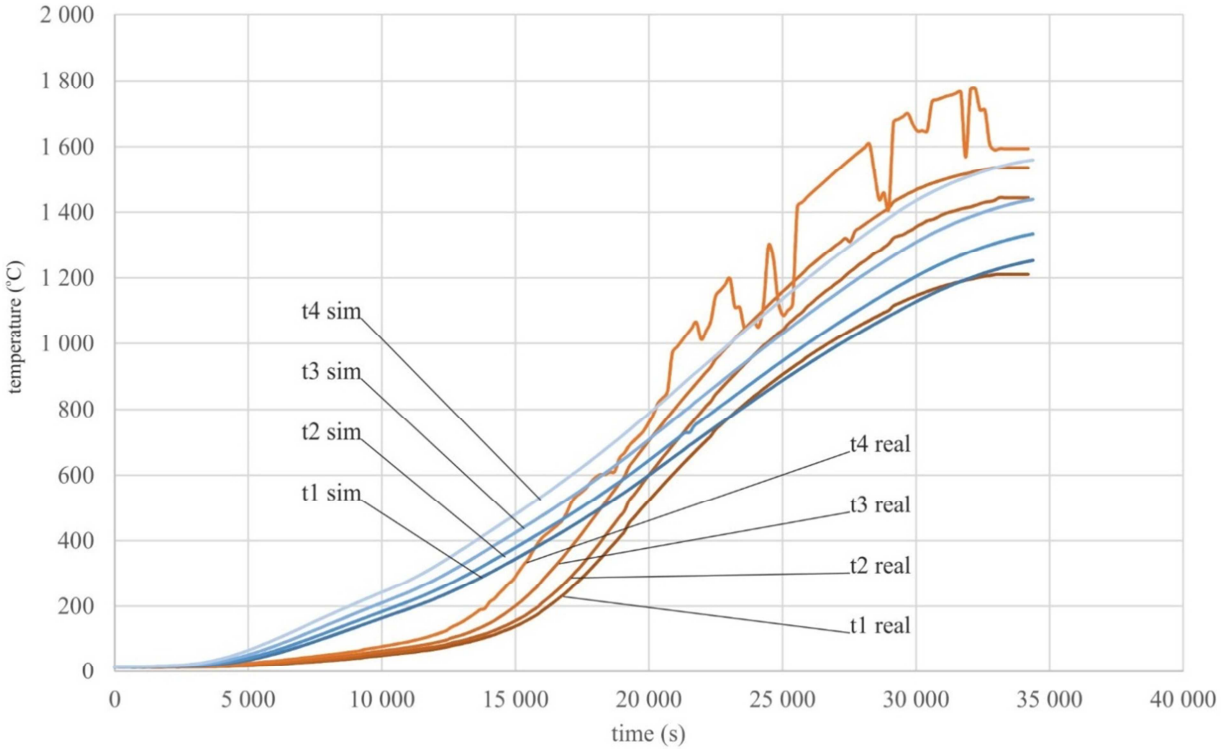

Figure 6. *Graphical comparison of simulated and measured temperatures.*

For the process of controlled crystal growth, it is advisable to know the property of thermal inertia of the crystallization device. This value can be determined by simulation comparing the times of temperature stabilization on the heater and in a measuring point t1 sim (Figure 7). In this case the difference is 12,500 seconds (3.5 hours). The temperature stabilization at measuring point t1 sim occurred after approx. 44,900 s. This needs to be verified experimentally, under the same conditions as in simulation. From the measurements so far it indicates that the stabilization of the temperature at the point t1 real occurs much sooner after about 32,500 s. Subsequently, the physical model can be modified to match the result of the simulation with the measured results.

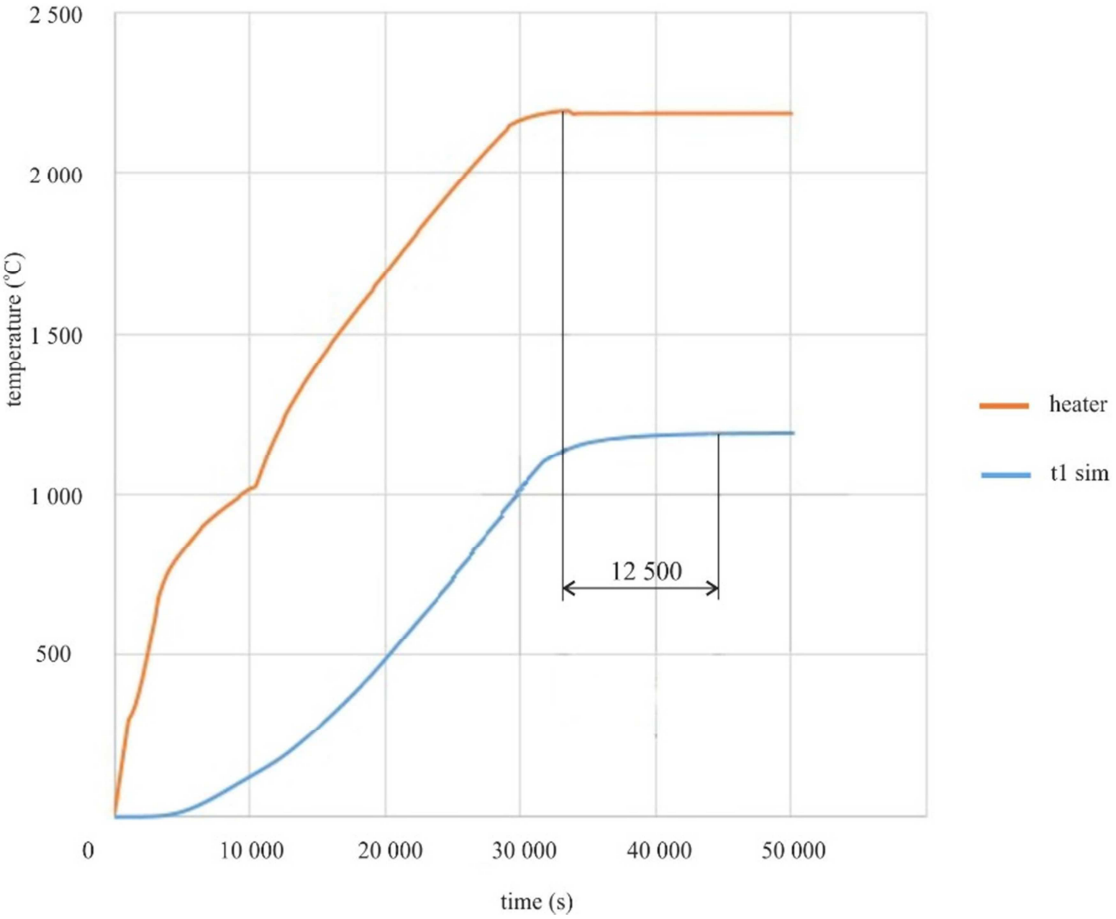

Figure 7. *Time difference stabilization of temperature on the heater and at the measuring point t1 sim.*

4. Conclusion

This simulation describes the dynamics of temperature fields in the structure of a heating unit during the start-up and run-up phase of the process. A verified physical model can be used to optimize the structure as well as the design of a new device and to optimize the crystallization process. The simulation has confirmed that the methodology and selection of the type of analysis are correct and the values of examined variables are close to the real ones. The next goal is to gradually refine the model and verify it. The final goal is to assemble a complete physical model with a melting container, raw material in both liquid and solid phase and a detailed heating unit design.

Acknowledgements

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