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TEMPERATURE DISTRIBUTION IN BRIDGMAN EQUIPMENT USED TO OBTAIN CALCIUM FLUORIDE SINGLE CRYSTALS

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Abstract
Calcium fluoride (CaF_2) single crystals have a very important role in optical applications. CaF_2 can be used in a wide region from ultraviolet to infrared. In IR applications it can be used as a prism, as spectroscopic windows and as lenses. The next generation of optical lithography is being driven by increased demand for faster and more powerful integrated circuits and calcium fluoride single crystals seems to be a very good solution for 193 and 157 nm technology. This paper present results concerning the temperature distribution in a Bridgman set-up used to obtain calcium fluoride single crystals. The numerical modeling of the entire set-up (global modeling) has been made using CrysVUn software and shows the influence of several parameters (heater geometry, screens position and geometry) on the temperature field, temperature gradient and on the solidification interface position.
Keywords: CaF_2, numerical modeling, temperature field.

1. Introduction

In order to optimize the Bridgman setup [1] used to obtain CaF_2 crystals and determining the optimum growth conditions, a series of numerical simulations have been performed using the CrysVUn software package. These simulations focused mainly on: determining the temperature distribution inside de growth setup, analysis of the shape and position of the solidification interface as a dependence of certain elements of the installation's construction, determining the temperature gradient in the hot area of the setup. Simulation results were correlated with experimental results and observations.

Numerical simulation plays a very important role in optimizing the components of a crystal growth setup as well as determining optimal growth conditions, necessary in order to obtain high quality crystals. The results of numerical modeling are even more relevant when they are backed up by experimental results. By using numerical simulation, one can establish a set of basic parameters for the actual growth process. Starting from a mathematical model that describes the physical process taking place inside the installation (a model that implies solving the equations that govern these processes), one can obtain results that are very close to reality. Numerical simulation also has an important advantage in reducing the time needed to investigate

different processes as well as overall project cost reduction when compared with the costs involved in doing an actual experiment.

2. Description of the Software

The software used in the investigation of the different physical phenomena that occur in a crystal growth process is called CrysVUn and it is being developed by the Crystal Growth Laboratory, Erlangen. CrysVUn is a global 2-D simulation of crystal growth inside complex setups that have axial or translational symmetries. It uses the finite volume method for computation and an unstructured grid. The results of the simulation supply information needed to make predictions about certain physical "variables" that are involved in the crystallization process. Global simulation must take into account all relevant physical phenomena that influence these variables. Temperature is the most important variable and is the basis for computing other variables such as thermal flux, flow speed, tensions inside the crystal.

A numerical simulation process has three main stages (steps) which are: - designing the geometry of the crystal growth setup; - determining the materials used and their characteristic constants and assigning them to different regions of the geometry; - setting the initial and border conditions and setting the parameters used for variable computation

CrysVUn contains modules that deal with each of these steps, more details being available in [2]. The software package described above is a product of the Crystal Growth Laboratory, Fraunhofer Institute IISB, Schottkystr. 10, 91058 Erlangen, Germany and is used by the Department of Physics at the West University of Timisoara through the good will of Prof. Dr. G. Muller, head of the equivalent department at Erlangen.

3. Results

The objective of this study is to determine the optimal growth conditions for a CaF_2:YbF_3 crystal. For this to be achieved, the temperature distribution within the entire growth setup, for different types of heater. The next step was the study of the shape and position of the solidification interface determined by a number of parameters (resistor shape, crucible position, screen position). The temperature distribution along the symmetry axis was also determined. The results obtained from the simulation have given some useful information which will be presented next and mentioned within the conclusion of this study. The physical properties of the material

used to define the different zones of the installation influence the results of the simulation substantially, especially results regarding heat transfer trough radiation and thermal conduction.

Material constants used where taken from specialist literature and trying to assure (as much as possible) that the data used where of recent date [3]. Table 1 shows the values for the materials that were considered. The initial and boundary conditions used are: initial conditions (initial temperature is 300K; electric power - varies from case to case); boundary conditions (the temperature on the outer walls of the installation (water cooled) is fixed at 300K; a "control point" is inserted in order to fixed the position of the solidification interface: position – (0, 0.639) with a corresponding temperature of 1673K - melting point for CaF_2)

Table 1: Material constants used.

	Property					
Material	Thermal conductivity (W/m*K)	Electric conductivity (S/m)	Heat capacity (J/kg*K)	Emissivity	Melting point (K)	Density (Kg/m^3)
Graphite	54		1770	0.95		2250
CaF_2	9.71	3189	880		1673	3200
Molybdenum	110	1.5*106	280	0.4		10000
Ceramics	1.8	0		0.13		

Fig. 1 presents the heater geometry and sketch (a), the set-up geometrical model (b) and the temperature distribution in the hot zone (c).

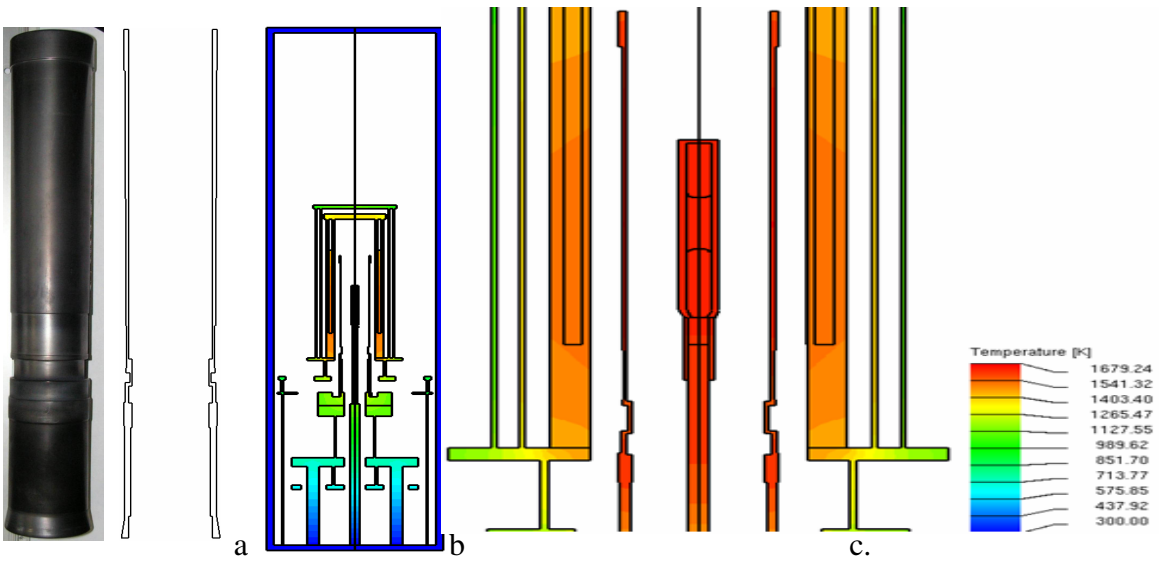

Fig. 1. a: Graphite heater. b, c: Temperature distribution in the set-up.

The temperature gradient along the symmetry axis was analyzed, in the case when the real heater geometry is used, both from the perspective of the numerical simulation results as well as from the point of view of experimental results and observations.

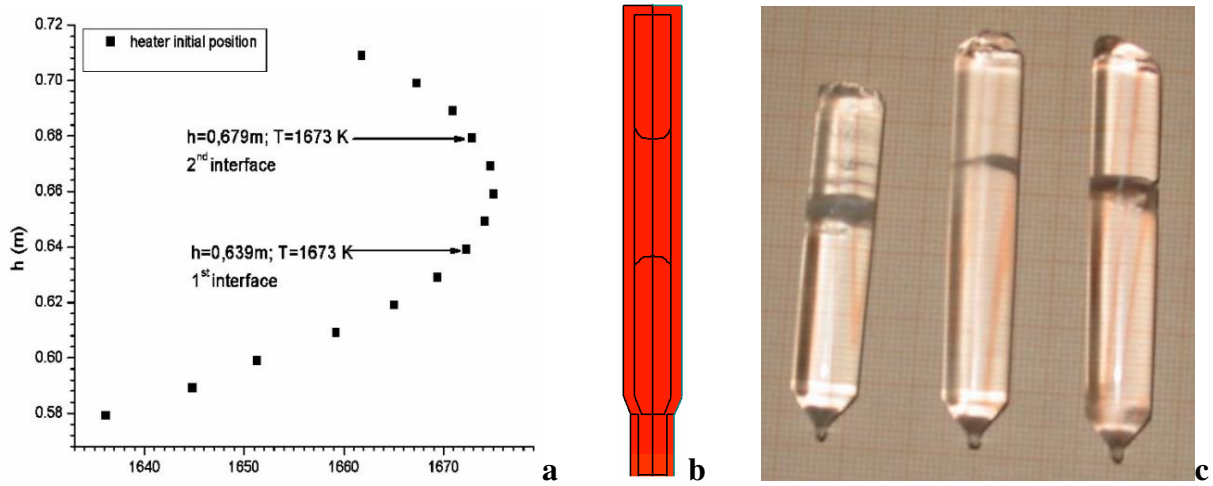

Fig. 2. a. Temperature gradient (within the crucible); b. The crucible and the solidification interface; c. CaF_2 crystals.

By analyzing the temperature gradient that was obtained by numerical simulation and also, from studying the graphical representation of the numerical results (Fig. 2a, b) it was observed that inside the crucible two interfaces are present corresponding to a temperature value of 1673K. The existence of the second, unwanted, interface was also observed experimentally (Fig. 2c). The result obtained via numerical simulation was exploited in order to eliminate the second interface which can be achieved by adjusting the growth setup geometry and modifying the initial position of the crucible within the temperature gradient.

In order to study the influence of the crucible position on the temperature distribution inside the crystal the case of the real heater and a crucible initially fixed at 194mm above the base of the heater was considered. The other two positions that were analyzed were the crucible lower by 30mm and 60mm below the initial reference position. By analyzing the temperature distribution within the hot zone, for each of the three distinct crucible positions, it was observed that by lowering the crucible by more then 30mm, the second solidification interface disappears. The power needed to assure optimum crystal growth conditions slightly decreases when lowering the crucible and the maximum temperature within the installation remains the same.

Fig. 3 presents the temperature distribution, along the symmetry axis, for 3 different positions of the crucible within the growth chamber. We can see that the crucible position has no significant influence on the temperature gradient near the solidification interface.

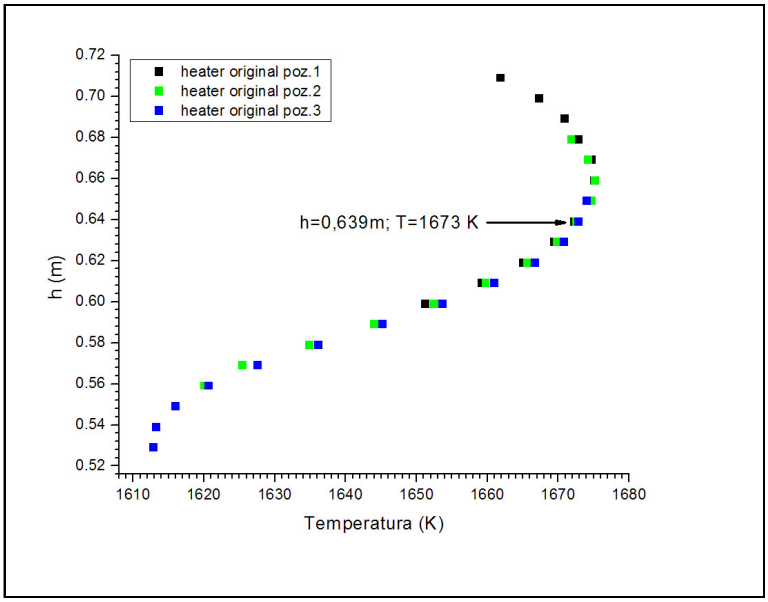

Fig. 3. Temperature distribution along the crucible symmetry axis.

Conclusions

- temperature distribution within the hot zone, in particular the temperature gradient along the symmetry axis, can be better controlled by using several independent heaters.
- the second, undesired, solidification interface which affects the quality of the obtained crystal in its superior part, was eliminated by modifying the geometry of the heater
- the parameters determined as a result of numerical simulation, made it possible to obtain an optimum temperature gradient (15K/cm) needed to obtain crystals of good quality.

References

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