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RESEARCH ARTICLE

Optimization of KRS-5 single crystal growth process by calculation of temperature gradient using finite element method

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Abstract

Objectives. Thallium halides, in particular KRS-5 (TlBr–TlI), represent one of the most promising classes of optical crystals for applications in the mid- and far-infrared ranges. Nevertheless, the high-quality standards applied to materials used for such applications present considerable challenges in the manufacture of single thallium halide crystals. In particular, when failing to adhere to exacting growth conditions, the samples exhibit polycrystalline characteristics, rendering them unsuitable for utilization. Given the high cost of experiments carried out to ascertain the optimal conditions for growth, computer modeling may present a viable alternative. When taking such an approach to satisfy the specific requirements, it becomes possible to analyze key effects as standalone entities, thus avoiding unnecessary complications resulting from the introduction of a high number of simultaneous unknown variables. Thus, the aim of the present work is to simulate the growth conditions of KRS-5 crystal to ascertain the causes of polycrystallinity in the samples and identify the optimal parameters for obtaining single crystals.

Methods. In order to solve the problem, the finite element method was used. This method is employed for the calculation of temperature distribution, mechanical stresses, convective effects, the rate of spreading of the crystallization front, deformations due to thermal expansion, and other phenomena that arise during the process of crystal formation. The MATLAB package, which includes a module for solving partial differential equations, was used to simulate the crystal growth ampoule. The problem of temperature gradient was solved in axisymmetric approximation.

Results. A computer simulation was employed to calculate the temperature distribution within the material during the growth process. This was used to determine the position and shape of the crystallization front. It is established that polycrystalline samples develop as a consequence of the crystallization front assuming a flat configuration. The optimum temperature in the furnace was determined. The work demonstrated the successful growth of a KRS-5 crystal under the calculated conditions.

Conclusions. The calculations used to identify the underlying cause of polycrystallinity in the samples enabled a determination of the optimal parameters for single crystal growth. On the basis of the calculations, a growth experiment was conducted on the KRS-5 sample. The obtained sample met the requisite criteria for commercial utilization.

Keywords

finite element method, temperature gradient calculation, optical crystals, thallium halide, KRS-5

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НАУЧНАЯ СТАТЬЯ

Оптимизация процесса роста монокристалла КРС-5 с помощью расчета градиента температуры методом конечных элементов

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Аннотация

Цели. Галогениды таллия, в частности, КРС-5 (TlBr–TlI), являются одними из наиболее перспективных оптических кристаллов среднего и дальнего инфракрасного диапазона. Однако высокие требования к качеству материала приводят к существенным сложностям производства данных монокристаллов, т.к. при несоблюдении точных условий роста образцы получаются поликристаллическими, непригодными для коммерческого использования. Для определения оптимальных условий роста необходимо проведение десятков дорогостоящих экспериментов. В таком случае альтернативным решением является компьютерное моделирование. В зависимости от требований можно анализировать ключевые параметры по отдельности, не усложняя модель множеством неизвестных одновременно. Целью данной работы является определение условий роста кристалла КРС-5 вычислительными методами для установления причин поликристалличности образцов и нахождения оптимальных параметров получения монокристаллов.

Методы. Для решения поставленной задачи использовали метод конечных элементов, с помощью которого можно выполнить расчеты температурного распределения, механических напряжений, конвективных эффектов, скорости распространения фронта кристаллизации, деформаций из-за теплового расширения и других явлений, возникающих в процессе кристаллообразования. Для построения модели ампулы использовался пакет MATLAB с модулем для решения уравнений в частных производных. Задача о температурном градиенте решалась в осесимметричном приближении.

Результаты. С помощью компьютерного моделирования рассчитано распределение температур в материале в процессе роста, на основе чего определено положение и форма фронта кристаллизации. Сделан вывод, что поликристалличные образцы растут в результате прохождения фронта кристаллизации плоской формы. Определена оптимальная температура в печи, необходимая для формирования выпуклого фронта кристаллизации. Продемонстрирован выращенный монокристалл КРС-5.

Выводы. Расчеты позволили быстро определить причину поликристалличности образцов, получить оптимальные параметры роста монокристаллов и на основе их провести эксперимент роста КРС-5. В полученном образце не наблюдалась блочная структура, и кристалл успешно подвергался механической обработке.

Ключевые слова

метод конечных элементов, расчет градиента температур, оптические кристаллы, галогенид таллия, КРС-5

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INTRODUCTION

Thallium halides exhibit uniform transparency across a broad wavelength range that encompasses the visible and mid-infrared regions from 0.35 to 50 μm. The transmission is up to 70% with a reflection coefficient of 30%. Absorption bands are not present within the transmission range. Depending on the composition, thallium halides are used in various fields. Among the thallium halides, KRS-5 crystals (Kristalle aus dem Schmelzfluss, German; 42.5% TlBr and 57.5% TlI) are the most promising for applications in space astrophysics, thermal imaging, and spectrophotometry. The crystals have mechanical, chemical, and vibrational strength and moisture resistance, which makes them suitable for use in atmospheric conditions without special protection. The combination of the characteristics of KRS-5 crystals has the potential to enhance the properties of equipment in the range of up to 10 μm, thereby providing a foundation for the development of novel devices operating in the range from 10 to 50 μm [1, 2].

Thallium bromide, a semiconductor with a band gap of 2.68 eV, is also promising. Due to its large atomic numbers (81 and 35) and high density (7.56 g/cm^3), it has excellent gamma radiation stopping ability [3, 4], which makes it ideal for detecting radiation at room temperature. Thallium bromide is also a promising material for positron emission tomography, as it provides very good energy resolution and the possibility of 3D segmentation, as well as detection efficiency superior to that of widely used scintillators [5, 6]. However, despite the good resolution of TlBr-based detectors, there is still instability in their operation. Attempts to solve this problem including adding iodine I or chlorine Cl atoms to the crystal [7], as well as doping with compensatory impurities [8, 9].

The growth of thallium halide crystals can be achieved using the Bridgman–Stockbarger method, which is particularly suited to the generation of single crystals of this composition [10]. Nevertheless, there are a number of problems in the production of these crystals, especially those having diameters over 50 mm. While key properties of these materials are their purity and structural perfection, methods for achieving material with an impurity content of no more than 10^{-5} wt % are not sufficiently worked out; consequently, the defect-free crystals often turn out to be far from perfect [11–13]. The technological process for obtaining single thallium halide crystals is additionally complicated by the toxicity of the material. The degree of polycrystallinity of the KRS-5 crystal significantly depends on the growth parameters in a multizone furnace. However, due to equipment wear, previously tested modes do not always provide the necessary quality of single crystals; the consequent search for new growth conditions through trial and error can entail unacceptable costs both in terms of expensive materials and time.

In this case, a computer simulation can serve as a solution [14]. Numerical methods have long proven themselves as an effective way to solve technological problems. When taking such an approach, it becomes possible to analyze key effects as standalone entities, thus avoiding unnecessary complications resulting from the introduction of a high number of simultaneous unknown variables. For example, calculations of temperature distribution, mechanical stresses, convection effects, propagation velocity of the crystallization front, deformations as a result of thermal expansion, as well as other phenomena occurring during crystal growth, are available within the framework of numerical methods. This work presents a solution to a simplified problem of searching for a temperature distribution to determine the growth parameters of high-quality crystal samples.

MATERIALS AND METHODS

All calculations were performed in the MATLAB package[1] using the Partial Differential Equation Toolbox (PDEs[2]) module for solving partial differential equations. The issue of temperature distribution was addressed by means of an axisymmetric approximation. The height of the ampoule model was 0.35 m, the radius was 0.04 m, and the angle at the tip of the cone was 45°C. The ampoule model was divided into a grid with triangular elements no larger than 0.005 m in size with a quadratic division of the grid nodes and a mesh growth rate of 1.5.

The following properties of the KRS-5 crystal were taken: heat capacity C = 151 W·s/(kg·°C), thermal conductivity k = 0.544 W/(m·°C), and density ρ = 7.37 g/cm^3 [15]. Crystal growth was carried out in *Giredmet* (Russia) from a charge comprising a compound of two salts of iodide and thallium bromide (*Giredmet*, Russia) in an EDG11-D4 Sunfire furnace (*MELLEN*, USA).

RESULTS AND DISCUSSION

The growth of single crystals of vertically directed crystallization can be achieved in a multizone furnace without the necessity for a membrane to separate the cold and hot zones. In this case, instead of moving the ampoule with the melt, it is possible to change the temperature of the heating elements and thereby shift the position of the crystallization isotherm (Fig. 1a).

A charge of the KRS-5 composition is placed in an ampoule made of heat-resistant glass, after which the ampoule is suspended inside the furnace (Fig. 1b). Subsequently, the temperature within the entire working area increases to a level above the melting point causing the material to enter a molten state. The temperature of the heating elements is then consistently reduced to values below the crystallization temperature of KRS-5, commencing with the elements situated beneath the ampoule containing the material. This subsequently results in the formation of a crystalline phase within the ampoule. However, the acquisition of high-quality samples relies on more comprehensive information pertaining to the growth parameters in question. For example, Fig. 1c shows a sample of polycrystalline KRS-5 obtained by maintaining a temperature gradient of up to 10°C/cm and a crystal

[1] MATLAB. version 9.14.0 (R2023a). Natick, Massachusetts: The MathWorks Inc.; 2023.

[2] Partial Differential Equation Toolbox. version 9.14 (R2023a). Natick, Massachusetts: The MathWorks Inc.; 2023.

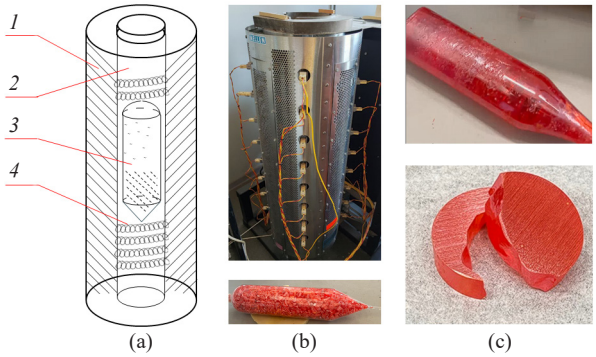

Fig. 1. (a) Schematic representation of a multizone furnace: (*1*) insulator; (*2*) working zone; (*3*) ampoule with KRS-5; (*4*) heating elements. The temperature of each heating element is regulated independently, allowing for the coexistence of the crystal phase and the melt within the ampoule (illustrated by dotted lines and waves). (b) Photo of a multizone furnace and an ampoule with powder that is suspended within the heating zone. (c) KRS-5 crystal grown in the furnace (photo above). If the temperature regime is not correct, the crystal falls apart during processing (photo below)

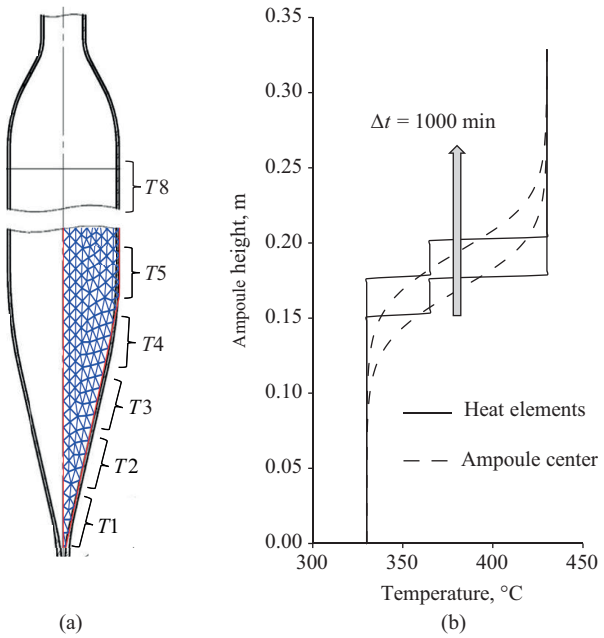

Fig. 2. (a) Model of the ampoule made of heat-resistant glass. The blue color shows the mesh. Each element has the properties of the KRS-5 material. The positions of the heating elements are indicated by T1–T8. (b) The temperature of the heating elements (solid line) and the corresponding temperature at the center of the flask (dashed line) at two points in time are illustrated. The arrow indicates where the dependencies shift over time

growth rate of no more than 1.5 mm/h. Since one of the key applications of KRS-5 is optics, the obtained samples are subsequently subjected to mechanical processing. Polycrystalline samples cannot withstand such processing and are therefore unsuitable. The growth of polycrystals may be attributed to a number of factors, including the shape of the crystallization front, stresses at the ampoule/material contact boundary, convection mechanisms, and the presence of multiple crystallization centers. Since the process of searching for a solution by selecting parameters is both costly and time-consuming, a decision was taken to employ numerical modeling.

In order to ascertain the shape of the crystallization front, it was considered to be sufficient to concentrate on the calculation of the isotherms within the ampoule, i.e., without considering convection or mechanical stresses at the interface between the material and the ampoule. Should the necessity arise, the latest effects may be incorporated into the complex model.

To carry out finite element modeling, an axisymmetric 2D model of an ampoule with a material was created in the MATLAB package, see Fig. 2a. As part of the task, the standard equation of thermal conductivity was solved:

$$\rho C_p \frac{\partial T}{\partial t} = \nabla(k \nabla T),$$

where T is the temperature; t is the time. The elements were given the characteristics of heat capacity (C_p), thermal conductivity (k) and density (ρ) corresponding to the KRS-5 crystal. Given that a sufficiently slow rate of crystal growth allows the system to reach thermal equilibrium, the effect of the heat of crystallization was not considered in the problem. The temperature of the heating elements was fixed at the edges of the model. The dimensions of the temperature-controlled sites and the size of the model were in accordance with the specifications of the experimental setup. The position of the crystallization front was further assumed to correspond to the position of the crystallization isotherm ($T_{cr} = 414$°C).

The temperature of the heating elements changed over time according to the following algorithm: first, the temperature of all heaters was equal to the maximum temperature: $T1 = T2 = ... = T8 = T_{max}$. Then the temperature of the first heater changed according to the ratio

$$T1 = T_{max} - \left(\frac{t - t_1}{1000 \cdot (T_{max} - T_{min})} \right),$$

where t_1 is the time of the start of cooling of the element $T1$ (min); t is the calculation time (min). After cooling the element $T1$ to T_{min}, the temperature on the element $T2$ was changed similarly. The temperatures T_{min} and T_{max} varied in different calculations in the ranges 330–360°C and 430–460°C. The profile of temperatures and heaters depending on height is shown in Fig. 2b. At these specified parameters, the crystallization isotherm exhibits a shift of 2.5 cm over the course of

1000 min, which corresponds to a crystal growth rate of 1.5 mm per hour.

Figure 3 shows the 3D surfaces of a part of the model having a temperature below the crystallization temperature of 414°C; a change in the shape of the isotherms is seen when the temperature of the heaters is switched both in the cone region and in the cylindrical region of the ampoule. Figures 3a and 3b show a comparison of two temperature regimes in which, at the same difference in maximum and minimum temperatures, a fundamentally different form of the crystallization isotherm is observed. If the range is shifted so that the maximum temperature is close to the crystallization temperature T_{cr}, the shape of the isotherm is convex (Fig. 3a). In the converse case, if the minimum temperature is close to T_{cr}, the shape of the crystallization isotherm is concave.

In quasi-stationary mode, when the growth rate is markedly slower than the rate of establishment of temperature equilibrium, it is postulated that the position of the crystallization front correlates with the crystallization isotherm. The morphology of the crystallization front exerts a considerable influence on the quality of the developing crystal. For example, according to studies conducted in the 20th century [16], the convex boundary of the crystallization front prevents the appearance of new nucleation centers on the path of further growth of the main crystal; this is due to the part of the crystal that has advanced into the melt being furthest from the walls, where the formation of new nuclei is most likely. It is also crucial to highlight that the ampoule cone is the area with the highest likelihood of defect growth. The greater the angle at the tip of the cone, the greater the probability of polycrystallinity. Therefore, the shape of the ampoule is of great importance, as it affects the probability of polycrystalline formation.

Furthermore, the degree of polycrystallinity exhibited by the crystal may be contingent upon the morphology of the crystallization front. Since polycrystallinity is often formed as a result of accumulation of dislocations, which move mainly perpendicular to the growth boundary, dislocations can be “pushed out” of the crystal with a convex front without creating a high density of defects [17]. Thus, in order to obtain high-quality samples, it is necessary to use the mode shown in Fig. 3a. From calculations, it is also possible to determine the magnitude of the gradient in the crystallization front zone. According to the isotherms at Figs. 3a and 3b, the gradient in the center of the ampoule is 11°C/cm for the first mode and 14°C/cm for the second.

According to the calculated regime, a new KRS-5 crystal was grown in a multizone furnace. The sample is presented in Fig. 3c. The quality control of the crystals was conducted through visual examination in well-illuminated conditions without the utilization of a microscope or other optical instruments. The observation was carried out at sharp angles to the surface of the samples. Under such inspection conditions, blocks due to imperfection of the crystal structure are visible. However, no block structure was observed in the obtained sample and the crystal was successfully machined.

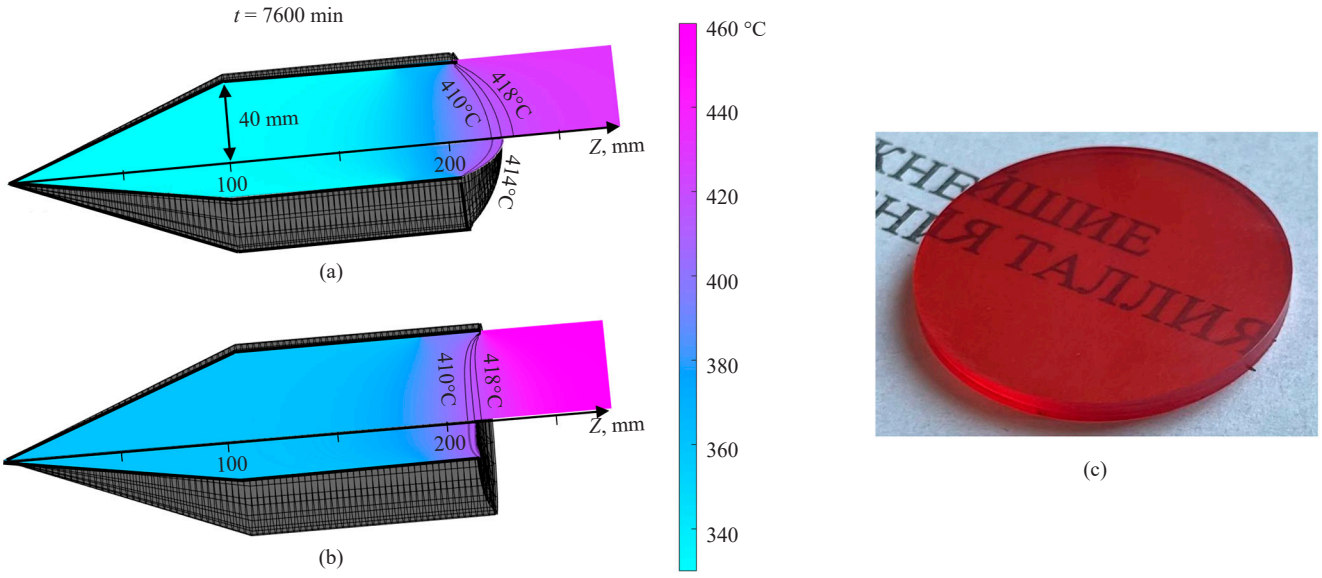

Fig. 3. (a), (b) 3D models of the crystallized part of the material inside the ampoule in the case of two temperature regimes: (a) 330–430°C; (b) 360–460°C. The color gradient shows the temperature distribution within the material. Three isotherms, for 410, 414, and 418°C, are marked with black lines. (c) Processed sample of KRS-5 crystal obtained using the temperature regime (a)

CONCLUSIONS

Using the finite element method implemented in the MATLAB package, the temperature distribution in a multizone furnace was obtained. Given that the crystallization front is located along the crystallization isotherm in the case of sufficiently slow crystal growth, it can be posited that the polycrystalline nature of previously grown crystals stems from the flat shape of the crystallization front, which, in turn, leads to the emergence of multiple crystallization centers, thus giving rise to a polycrystalline structure. Subsequently, new growth parameters were established to set the corresponding temperature values on the heating elements, thereby enabling the growth of a KRS-5 crystal with a low degree of polycrystallinity, which is suitable for commercial use.

Authors' contributions

S.V. Erohin—carrying out calculations, writing the text of the article.

K.S. Zaramenskikh—developing growth regimes, writing the text of the article.

M.S. Kuznetsov—growing crystals in a multizone furnace, planning the experiment.

S.M. Pilyushko—preparing samples and mechanical processing.

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