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USE OF COMPUTER SIMULATION FOR OPTIMIZATION OF TECHNOLOGICAL MODES OF MANUFACTURING THERMOELECTRIC MATERIALS BASED ON *Bi-Te* OBTAINED BY VERTICAL ZONE MELTING METHOD

The article presents the main types of computer models used for the study of thermoelectric materials. A description of physical and mathematical models of crystal growth, and a method of using crystal growth models to optimize the technology of manufacturing thermoelectric material based on Bi-Te, and thermoelectric parameters of manufactured thermoelectric materials are given. Bibl. 5. Fig. 4.

Key words: vertical zone melting, thermoelectric material, computer model.

Introduction

In the age of technological progress and high requirements to production efficiency, computer simulation is becoming an indispensable tool for the development and improvement of new materials and technologies. One of the areas where this is especially relevant is the production of thermoelectric materials by the method of vertical zone melting, since this method is the main one in the mass production of thermoelectric products [1 – 2]. The advantages of using computer simulation in this context are obvious and tangible at every stage of thew process.

The relevance of the work is the introduction of computer methods into the technological modes of manufacturing thermoelectric materials, which will reduce materials costs and time for the process of improving the material.

The purpose of the work is to develop a computer approach for optimizing technological modes for the production of thermoelectric materials

Computer models in thermoelectricity

The main types of models used in the research of thermoelectric materials are:

- Kinetic models: These models describe the dynamics of crystal growth according to the laws of physical chemistry and heat transfer. They take into account diffusion processes, mass transfer, heat transfer, etc.
- Flux models: These models investigate the movement and interaction of atoms or molecules in the melt phase, specifically accounting for the flux of reactants and products.
- Molecular dynamics: In these models, atoms or molecules are considered individually and their motions are modeled using physical laws.

- Computer simulation of mass and heat transfer: These models describe the interaction of reagents with the surface of the crystal, diffusion processes, heat flows, etc.

Crystal growth models: These models study crystal growth by considering various process parameters such as temperature, growth rate, reactant concentration.

Description of the computer model

The use of computer models of crystal growth is the most promising solution for optimizing the technological regime for growing thermoelectric material. These models take into account various parameters and conditions for crystal growth, such as temperature, growth rate, and concentration of reagents. They are based on the physical principles of diffusion, heat transfer and other processes that occur during zone melting. These models can provide information about how the crystallization front moves, what factors affect its shape and speed of formation. The shape of the crystallization front is one of the key parameters that affects the quality of the obtained thermoelectric material. The most favorable for the growth of single crystals with a small number of structural defects is a flat crystallization front, because on the crystallization front convex in the melt or concave in the crystal, random crystal nuclei (impurity nuclei) will grow compatible with the main one, and on the flat crystallization front, uniform and stable crystal growth is formed with a minimum number of defects [3 – 5].

Based on the physical model of vertical zone melting, a computer model was created to study the formation of the shape of the crystallization front in order to find the optimal dimensions of the heater for a specific thermoelectric material based on *Bi-Te*. The physical model of vertical zone melting is presented in Fig. 1.

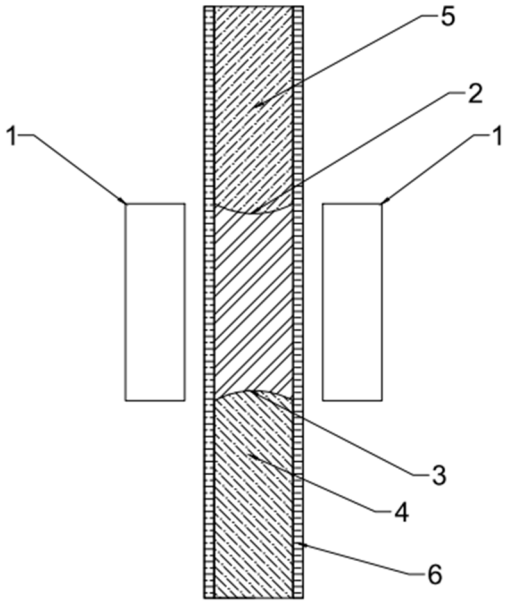

Fig. 1. Physical model: 1 –heaters, 2 – boundary of melt front,
3 – boundary of crystallization front, 4 – material in solid phase (single crystal),
5 – material in solid phase (polycrystal), 6 – quartz ampoule

The computer model was created using Comsol Multiphysics software. It represents a classical system of differential equations of thermal conductivity supplemented by dependences of the physical properties of the material being studied. The constructed computer model makes it possible to change

geometric and temperature parameters and monitor the formation of the crystallization front. The results of modeling the dependence of the shape of the crystallization front, thermoelectric material based on *Bi-Te*, on the height of the cylindrical heater are shown in Fig. 2. This made it possible to determine that the flat front is fully formed at the ratio $h = 2.25d$ for the given composition of the thermoelectric material based on *Bi-Te*. To determine the influence of the shape of the crystallization front on the parameters of this thermoelectric material based on *Bi-Te*, two ingots were made, the first with a ratio of $h = 2.25d$, and the second with $h = 1.5d$. The thermoelectric parameters of the manufactured material are presented in Fig. 3, 4.

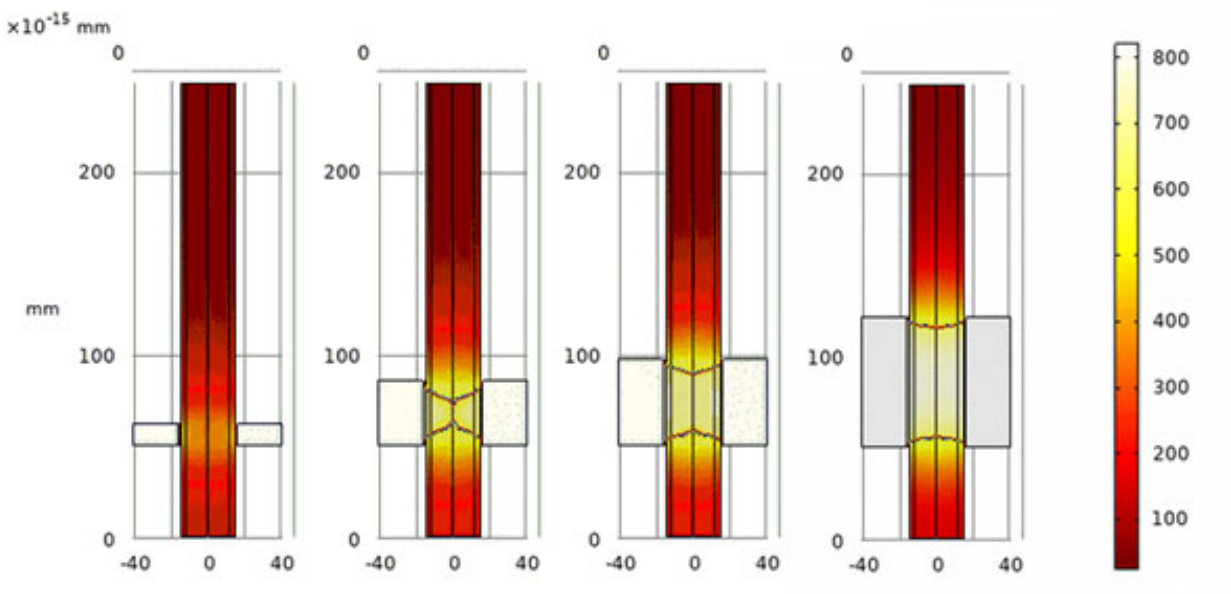

Fig. 2. Computer model of change in the shape of crystallization front

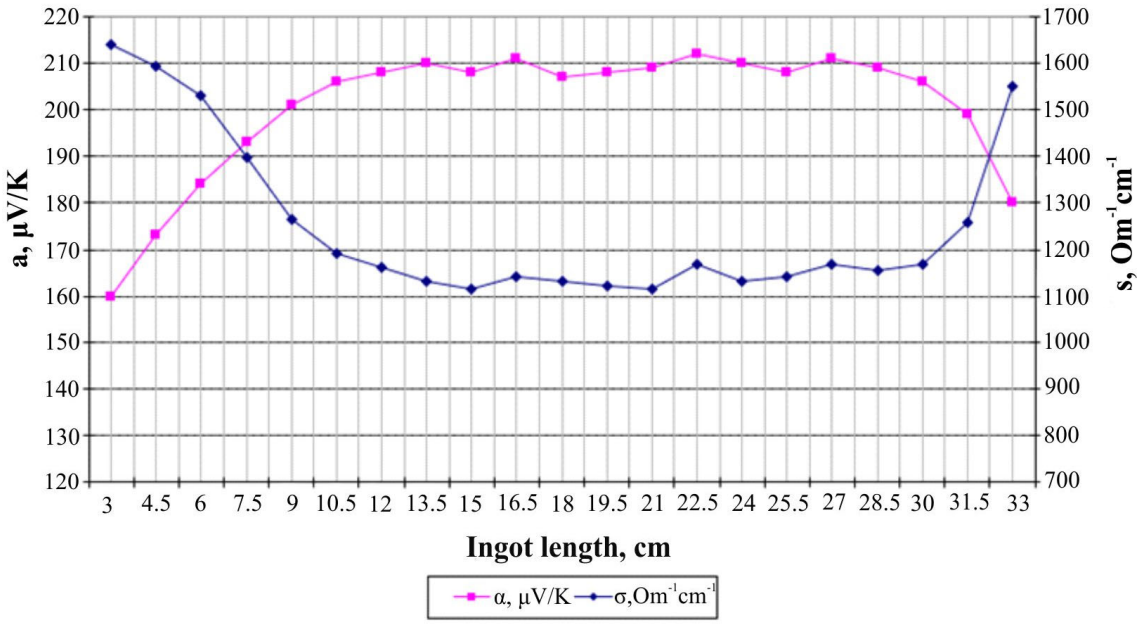

Fig. 3. Thermoelectric parameters, where h=2.25d

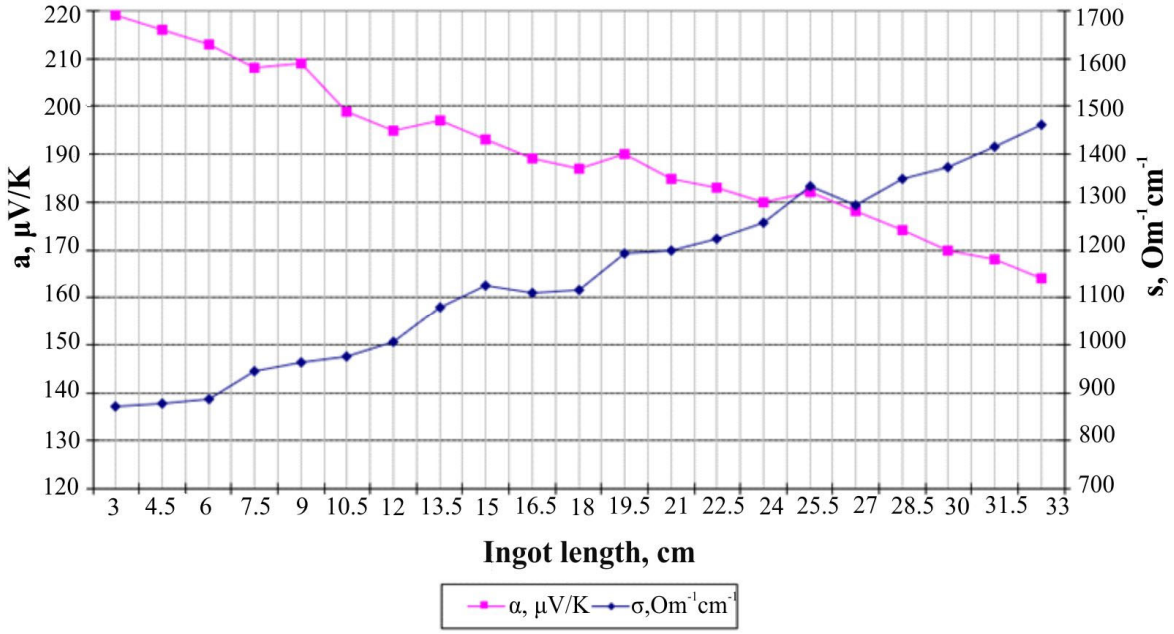

Fig. 4. Thermoelectric parameters, where h=1.5d

As can be seen from the graphs, a flat crystallization front and a relatively large volume of the liquid phase (h = 2.25d) create a homogeneous material with a small number of structural defects along the entire length of the ingot, while the material obtained at a ratio of h = 1.5d, is characterized by heterogeneity of thermoelectric parameters along the length of the ingot. Since nowadays there is a tendency to increase the volume of material production by increasing the diameter of ampoules, the known ratios calculated in other works do not always retain their relevance. That is why it is expedient to study the conditions for the formation of a flat crystallization front, for each composition of components of a thermoelectric material, as a preparatory stage of the technological process, this is especially relevant for the mass production of thermoelectric materials at enterprises.

It should be noted that depending on the composition of the components, or when the technological equipment is changed, the period of formation of the flat crystallization front may also change, which will require additional research to optimize the new technology and maximize the quality of the manufactured thermoelectric material. Such studies usually lead to significant expenditure of time and money for conducting experiments, therefore, the use of such computer models for the optimization of this process allows to significantly reduce the material costs and time required for the optimization of the manufacturing technology.

Conclusions

The use of computer simulation in the production of thermoelectric materials obtained by the method of vertical zone melting allows for a faster, more efficient and innovative development and manufacturing process. This significantly reduces the time and material costs of experiments and opens up new opportunities for the creation of highly efficient materials thar can be widely used in the production of thermoelectric devices and systems that use renewable energy sources and heat flows.

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ВИКОРИСТАННЯ КОМП'ЮТЕРНОГО МОДЕЛЮВАННЯ ДЛЯ ОПТИМІЗАЦІЇ ТЕХНОЛОГІЧНИХ РЕЖИМІВ ВИГОТОВЛЕННЯ ТЕРМОЕЛЕКТРИЧНИХ МАТЕРІАЛІВ НА ОСНОВІ *Bi-Te* ОТРИМАНИХ МЕТОДОМ ВЕРТИКАЛЬНОЇ ЗОННОЇ ПЛАВКИ

У статті наводяться основні типи комп'ютерних моделей, які застосовуються для дослідження термоелектричних матеріалів. Наводиться опис фізичної та математичної моделей вирощування кристалів, та метод застосування моделей вирощування кристалів для оптимізації технології виготовлення термоелектричного матеріалу на основі Bi-Te, та термоелектричні параметри виготовлених термоелектричних матеріалів. Бібл. 5. Рис. 4.
Ключові слова: вертикальна зонна плавка, термоелектричний матеріал, комп'ютерна модель.

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