used [5]. The model employs the hydrodynamic theory, where a material is regarded as a fluid of high viscosity which is a function of velocity and temperature. The internal friction of the moving layers of material serves as a heat source. The developed computer model allows one to determine mechanical stress distribution in the matrix due to external pressure and thermal loads.

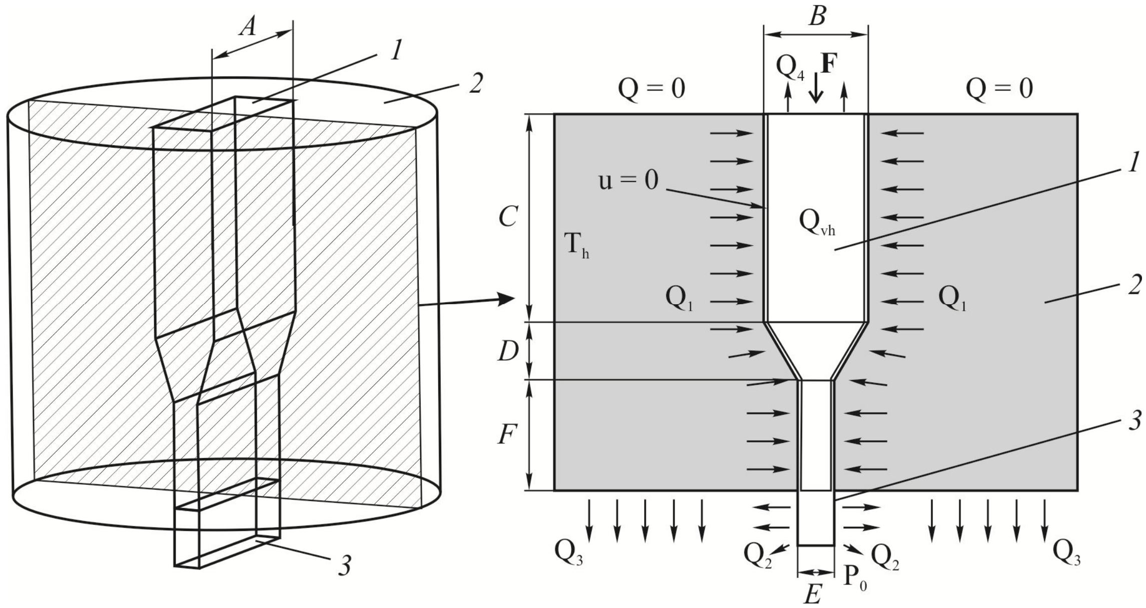

Fig. 1. Physical model of the extrusion process of tape thermoelectric material.
1 – thermoelectric material billet; 2 – matrix; 3 – tape thermoelectric material after leaving the matrix.

The employed physical model of the extrusion process of tape material is shown in Fig. 1. The model considers a stationary case of flowing through matrix 2 of material billet 1 obtained by cold pressing. The geometrical dimensions: *A*, *B* and *C* are width, thickness and length of matrix inlet (thermoelectric material billet); *D* is the length of the beveled part of the matrix; *E*, *F* are the thickness and length of matrix outlet whose width is *A*.

To find the distributions of velocities and temperatures, one should solve the following system of equations [5]

$$\rho(\boldsymbol{u}\cdot\nabla\boldsymbol{u}) = \nabla\left[-p\boldsymbol{I} + \eta(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T) - \frac{2}{3}\eta(\nabla\cdot\boldsymbol{u})\boldsymbol{I}\right] + \boldsymbol{F}\ ;$$

$$\nabla\cdot(\rho\boldsymbol{u}) = 0\ ; \qquad (1)$$

$$\rho C_p \boldsymbol{u}\cdot\nabla\boldsymbol{T} = \nabla\cdot(\kappa\nabla T) + Q_{vh}\ ;$$

$$Q_{vh} = \eta(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T - \frac{2}{3}(\nabla\cdot\boldsymbol{u})\boldsymbol{I}) : \nabla\boldsymbol{u}$$

with the corresponding boundary conditions:

– thermostated lateral surface of matrix: $T = T_h$,
– convective heat exchange of the lateral surface of sample after leaving the matrix:

$$-\boldsymbol{n}\cdot(-\kappa\nabla T) = h_2(T - T_0)\ ,$$

– heat removal by structural members, not shown in Fig.1, from lower matrix part and upper part of thermoelectric material billet:

$$-\boldsymbol{n}\cdot(-\kappa\nabla T)=h_3(T-T_0)\,,\ -\boldsymbol{n}\cdot(-\kappa\nabla T)=h_4(T-T_0)\,,$$

– thermal insulation of upper matrix part:

$$-\boldsymbol{n}\cdot(-\kappa\nabla T)=0\,,$$

– input pressure on the billet: $p = p_1$,
– atmospheric pressure at sample exit from the matrix: $p = p_0 = 1$ atm.,
– equality to zero of fluid velocity at the boundary of contact with the matrix $\mathbf{u} = 0$,
– equality to zero of fluid velocity component perpendicular to the lateral side of the sample after leaving the matrix $\mathbf{u_n} = 0$,

where: $\boldsymbol{u}$ is velocity field, ρ is density, p is pressure, η is dynamic viscosity factor, κ is thermal conductivity, $\boldsymbol{F}$ is vector field of forces, Qvh is volumetric heat source due to internal friction, $\boldsymbol{I}$ is unit matrix, h_2 - h_4 are heat exchange coefficients, T_0 is ambient temperature.

Heating due to internal friction and contact thermal resistance at the boundary of contact between material and matrix are taken into account. The properties of thermoelectric material and matrix material used in simulation are given in Table 1.

Table 1.

Material properties

1.	Thermoelectric material	Thermal conductivity, W/(m*K)	4
		Density, kg/ m^3	7600
		Heat capacity, J/(kg*K)	150
2.	Steel (matrix)	Thermal conductivity, W/(m*K)	24.3
		Density, kg/ m^3	7850
		Heat capacity, J/(kg*K)	500

Equivalent viscosity of test fluid and other parameters necessary for computer model are calculated by the formulae given in [6].

Fig. 2 shows a mesh of finite element method which is used in Comsol Multiphysics for matrix configuration under study.

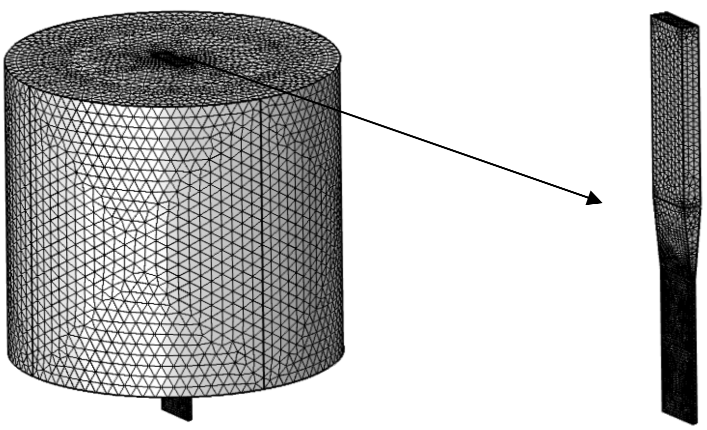

Fig. 2.Finite element method mesh built for matrix configuration shown in Fig. 1.

Computer simulation results

Typical velocity fields and temperature distributions in the matrix and thermoelectric material obtained by computer simulation are shown in Figs. 3, 4. The velocity in mm/min and temperature in degrees Celsius are marked in colour.

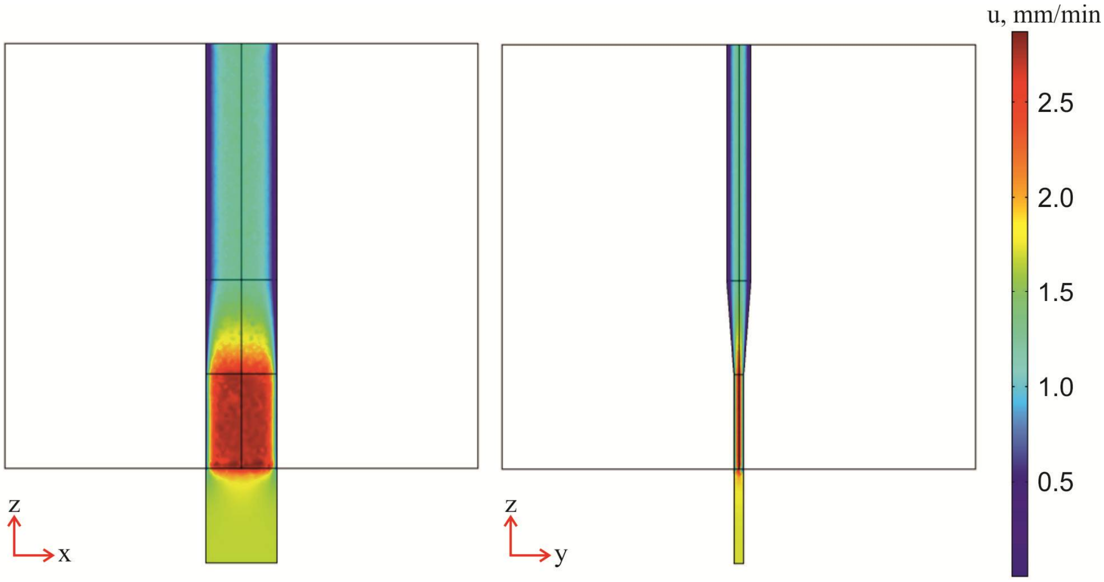

Fig. 3.Velocity field of thermoelectric material inside the matrix and after leaving it (for matrix with dimensions: A = 15mm; B = 5 mm; C = 50 mm; D = 20 mm; E = 2 mm; F = 20 mm).

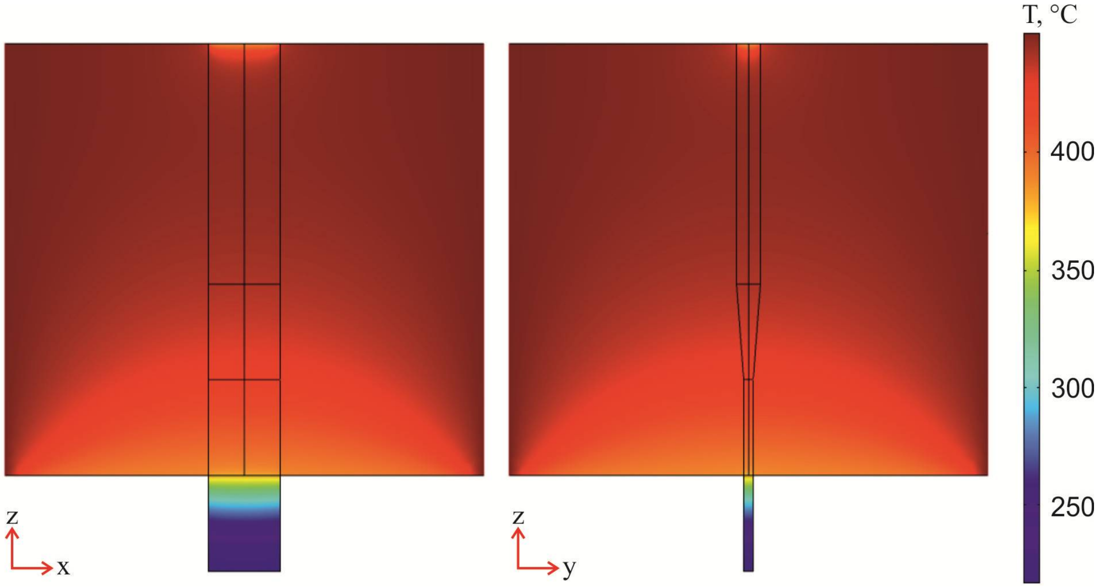

Fig. 3.Temperature distributions in thermoelectric material and matrix (for matrix with dimensions: A = 15mm; B = 5 mm; C = 50 mm; D = 20 mm; E = 2 mm; F = 20 mm).

Fig. 4 shows velocity fields in thermoelectric material at the exit from matrix obtained for various matrix configurations – its inlet and outlet dimensions (indicated in the figure in mm).

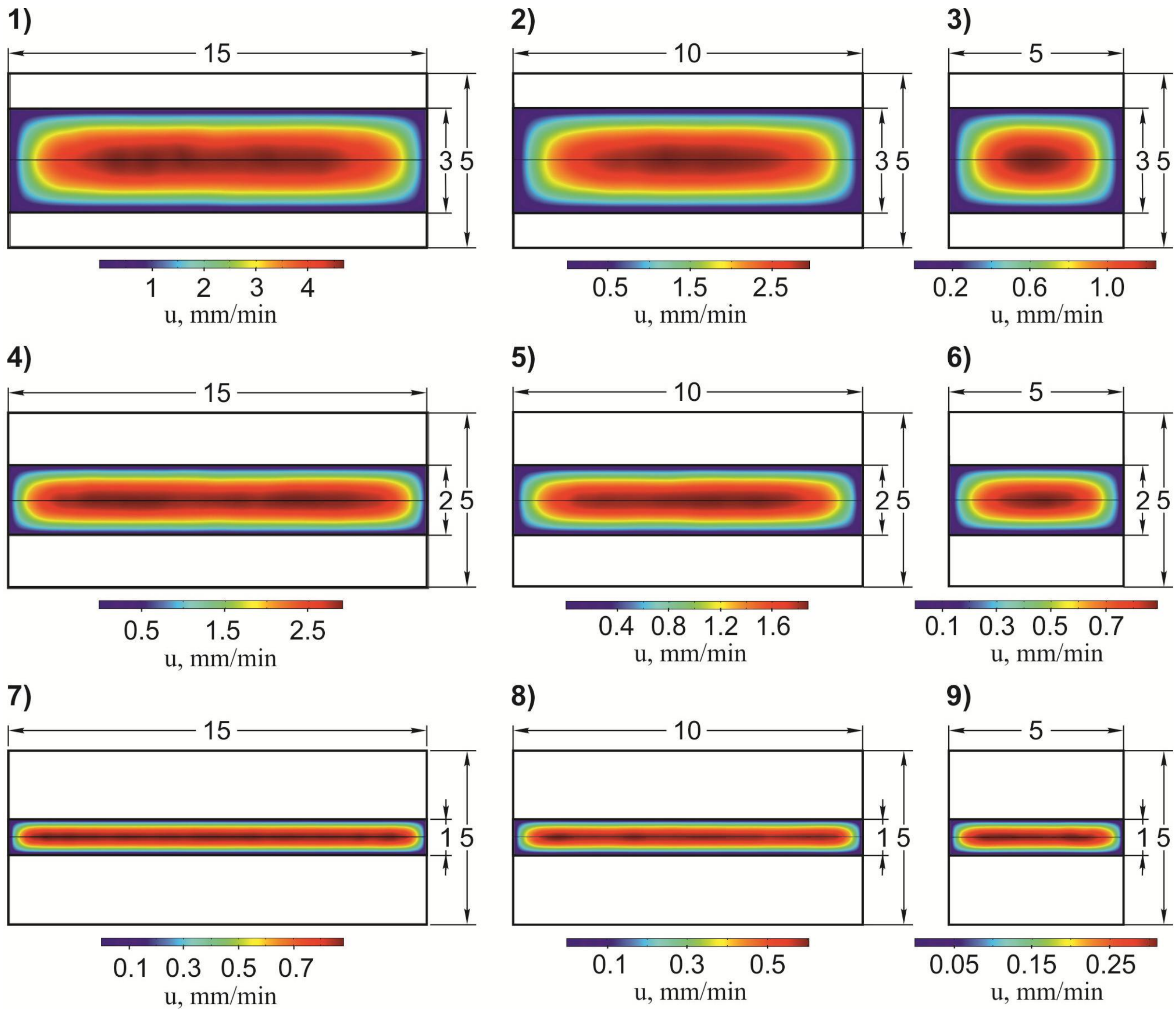

Fig. 4.Velocity fields in thermoelectric material at the exit from matrix obtained for various matrix configurations.
1 – A = 15 mm, B = 5 mm,, E = 3 mm, 2 – A = 10 mm,, B = 5 mm,, E = 3 mm,;
3 – A = 5 mm,, B = 5 mm,, E = 3 mm,; 4 – A = 15 mm,, B = 5 mm,, E = 2 mm,;
5 – A = 10 mm, B = 5 mm, E = 2 mm,; 6 – A = 5 mm,, B = 5 mm,, E = 2 mm,;
7 – A = 15 mm, B = 5 mm, E = 1 mm; 8 – A = 10 mm, B = 5 mm, E = 1 mm;
9 – A = 5 mm, B = 5 mm, E = 1 mm.

Fig. 5 shows velocity distributions along the width of the output tape thermoelectric material (1 mm after leaving the matrix). In the percentage ratio, the smallest velocity spread is typical for cases with the largest thickness ratio of matrix inlet and outlet.

Since extrusion conditions, i.e. die shape, temperature and strain rate, etc., directly affect the final structure and properties of the extruded material, the information obtained is useful for optimizing the design of equipment for extrusion of *Bi-Te* based tape materials. The computer model developed can also, if necessary, reproduce these results for other materials and extrusion conditions.

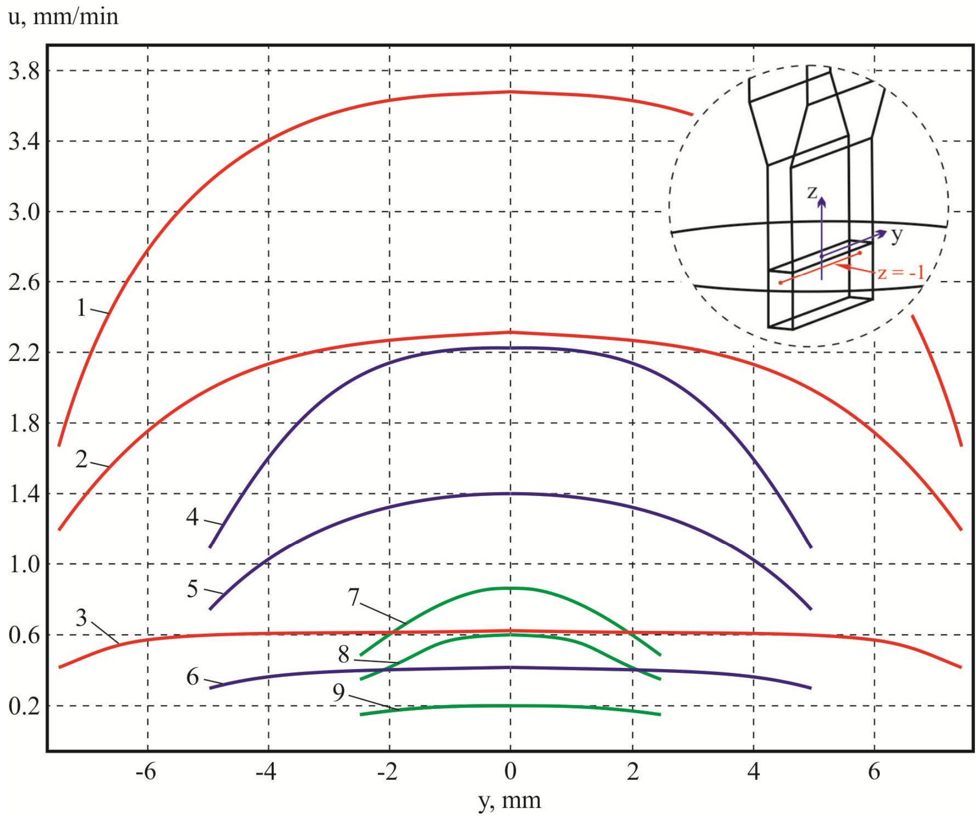

Fig. 5. Velocity distributions along the width of the output tape thermoelectric material (1 mm after leaving the matrix) for various matrix geometry:1 – A = 15 mm, B = 5 mm, E = 3 mm; 2 – A = 15 mm, B = 5 mm, E = 2 mm; 3 – A = 15 mm, B = 5 mm, E = 1 mm; 4 – A = 10 mm, B = 5 mm, E = 3 mm; 5 – A = 10 mm, B = 5 mm, E = 2 mm; 6 – A = 10 mm, B = 5 mm, E = 1 mm; 7 – A = 5 mm, B = 5 mm, E = 3 mm; 8 – A = 5 mm, B = 5 mm, E = 2 mm; 9 – A = 5 mm, B = 5 mm, E = 1 mm.

Conclusions

1. A computer model of the hot extrusion process of Bi_2Te_3 based thermoelectric material was created which can be used to study the distributions of temperature and material flow velocity in the matrix, as well as mechanical stress distribution in the matrix due to external pressure and thermal loads.
2. The temperature and material flow velocity distributions in the matrix were obtained depending on matrix configuration for the case of thermoelectric material extrusion in the form of tape structures.
3. Dependences of velocity distribution of tape thermoelectric material after leaving the matrix were obtained versus size ratio of matrix inlet and outlet. Conditions for approximation of this distribution to the one-dimensional were determined.

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КОМП'ЮТЕРНЕ МОДЕЛЮВАННЯ ПРОЦЕСУ ЕКСТРУЗІЇ СТРІЧКОВИХ ТЕРМОЕЛЕКТРИЧНИХ МАТЕРІАЛІВ НА ОСНОВІ Bi_2Te_3

Оскільки в процесі гарячої екструзії термоелектричних матеріалів у вигляді стрічкових структур заготовки матеріалу деформуються в практично ідеальних пластичних умовах, при оптимізації обладнання для отримання таких матеріалів може бути використано наближення в'язкої рідини. Це дозволяє проводити комп'ютерне моделювання процесу екструзії з використанням теорії гідродинаміки, де матеріал розглядається як рідина з дуже високою в'язкістю, яка залежить від швидкості і температури. У роботі наведено результати об'єктно-орієнтованого комп'ютерного моделювання процесу гарячої екструзії термоелектричного матеріалу на основі Bi_2Te_3. Розглянуті випадки отримання термоелектричних матеріалів у вигляді стрічкових структур для різних конфігурацій матриці. Отримано розподіли температури та швидкості протікання матеріалу у матриці, а також поля швидкостей матеріалу на виході з матриці, які безпосередньо впливають на структуру отриманого матеріалу та його термоелектричні властивості. Бібл. 6, рис. 5, табл. 1.
Ключові слова: моделювання, екструзія, стрічковий термоелектричний матеріал.

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КОМПЬЮТЕРНОЕ МОДЕЛИРОВАНИЕ ПРОЦЕССА ЭКСТРУЗИИ ЛЕНТОЧНЫХ ТЕРМОЭЛЕКТРИЧЕСКИХ МАТЕРИАЛОВ НА ОСНОВЕ Bi_2Te_3

Поскольку в процессе горячей экструзии термоэлектрических материалов в виде ленточных структур заготовки материала деформируются в практически идеально пластических условиях, при оптимизации оборудования для получения таких материалов может быть использовано приближение вязкой жидкости. Это позволяет проводить компьютерное моделирование процесса экструзии с использованием теории гидродинамики, где материал рассматривается как жидкость с очень высокой вязкостью, которая зависит от скорости и температуры. В работе приведены результаты объектно-ориентированного компьютерного моделирования процесса горячей экструзии термоэлектрического материала на основе Bi_2Te_3. Рассмотренные случаи получения термоэлектрических материалов в виде ленточных структур для разных конфигураций матрицы. Получены распределения температуры и скорости протекания материала в матрицы, а также поля скоростей материала на выходе из матрицы, которые непосредственно влияют на структуру полученного материала и его термоэлектрические свойства. Библ. 6, рис. 5, табл. 1.

Ключевые слова: моделирование, экструзия, ленточный термоэлектрический материал.

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COMPUTER RESEARCH ON THE INFLUENCE OF THE PELTIER EFFECT ON THE CRYSTALLIZATION PROCESS OF Bi_2Te_3 BASED THERMOELECTRIC MATERIALS

The article presents the results of computer simulation of the process of growing Bi_2Te_3 based thermoelectric materials by the vertical zone melting method with regard to the Peltier effect occurring at the interface between solid and liquid phases of the grown material when electric current is passed through an ingot. Bibl. 7, Fig. 6, Tabl. 1.

Key words: simulation, vertical zone melting, thermoelectric material, growing in electric field.

Introduction

Bismuth telluride-based solid solutions are unique commercially available thermoelectric materials (TEM) for solid-state cooling and generation of electrical energy. Therefore, much attention is paid to the improvement of Bi_2Te_3 based TEM production methods.

Zone melting is one of the most used methods for the production of semiconductor materials, in particular thermoelectric. However, the production of thermoelectric materials with the necessary properties is possible only under the conditions of a controlled crystallization process, since when TEM is obtained by this method, the crystallization front curvature, the temperature gradient at the interface between the solid and liquid phases, the melt zone geometry, and the velocity have a great influence on the single crystal growth stability and homogeneity.

In [1-3], the possibility of growing single crystals of thermoelectric materials by the method of vertical zone melting in the presence of electric current passing through an ingot was considered. It is known that when passing an electric current, at the interface between the solid and liquid phases of the same semiconductor, just as at the interface between two different materials, the Peltier heat will be released or absorbed. This amount of heat is sufficient to affect the course of crystallization. However, studies of temperature distributions and geometry of the crystallization front cause considerable experimental difficulties, so simulation of the TEM growth process is relevant, which makes it possible to optimize the choice of technological parameters of the setup and the modes of material growth.

So, *the purpose of this work* is computer research on the influence of the Peltier effect that occurs at the interface between the solid and liquid phases when growing Bi_2Te_3 based thermoelectric materials by the vertical zone melting when passing electric current through the molten zone, on growing process, specifically, on the shape of crystallization front and temperature gradients.