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VISCOUS FLUID APPROXIMATION WHEN SIMULATING Bi_2Te_3 BASED THERMOELECTRIC MATERIAL EXTRUSION PROCESS

In the process of extrusion, billets of material are deformed under virtually perfect plastic conditions. Such a process can be simulated using the hydrodynamic theory, where a material is regarded as a fluid of very high viscosity which is a function of velocity and temperature. The internal friction of the moving layers of the material serves as a heat source, so it is also necessary to use the heat transfer equation in conjunction with the hydrodynamic aspect of the problem. This approach is especially effective for simulating the extrusion process of thermoelectric materials when large deformations are present. This paper presents the results of an object-oriented computer simulation of the process of hot extrusion of Bi_2Te_3 based thermoelectric material. Cases of producing cylindrical samples of circular cross section for various matrix configurations for single-stage and multi-stage extrusion are considered. The distributions of temperature and flow velocity of material in the matrix are obtained, as well as stress distribution in the matrix due to external pressure and thermal loads, which formed the basis for optimization of equipment for producing extruded thermoelectric material. Bibl. 5, Fig. 8, Tabl. 1.

Key words: extrusion, thermoelectric material, modeling.

Introduction

The hot extrusion process is widely used in the production of thermoelectric materials [1 – 3]. The essence of it is punching a thermoelectric material through a hole in a heated mold. The main advantage of this method is associated with an improvement in the strength characteristics of material. Moreover, their thermoelectric properties can remain at the level of the properties of materials obtained by crystallization from the melt.

Since hot extrusion is usually carried out at sufficiently high temperatures, the structure of the extruded material is formed in the process of plastic deformation, resulting in a deformation texture. The extrusion conditions, namely the shape of the die, the temperature and strain rate, the strain value, the structure of the initial billet, affect the final structure and properties of the extruded material. One of the effective ways to study the influence of these conditions on the formation of the structure and texture of the extruded material is mathematical simulation of the extrusion process in combination with the experimental results of structural studies [4].

The purpose of this work is to create a computer model of the hot extrusion process of Bi_2Te_3 based thermoelectric material to study the distributions of temperature and material flow velocity in the matrix, as well as the stress distribution in the matrix due to external pressure and thermal loads, which can be the basis for optimization of equipment for producing extruded thermoelectric material.

Physical, mathematical and computer extrusion models

To build a computer model of the hot extrusion process, the application package of object-oriented simulation Comsol Multiphysics was used [5]. In extrusion processes, the initial billets of material are deformed in a hot solid state under practically ideal plastic conditions. Such processes can be simulated using 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; therefore, heat transfer equations are also used in conjunction with the hydrodynamic aspect of the problem. This approach is especially effective for simulating the extrusion of thermoelectric materials in the presence of large strains. In addition, the developed computer model allows one to determine stress distribution in the matrix due to external pressure and thermal loads.

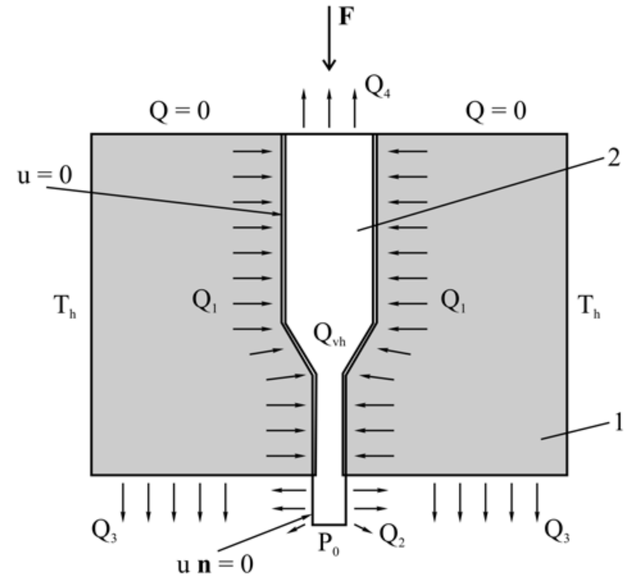


Fig. 1. Physical model of extrusion process

The physical model of the extrusion process is shown in Fig. 1. The model considers the stationary case of flow through matrix 1 of the cylindrical billet of material 2 obtained by cold pressing.

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

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

$$\nabla\cdot(\rho u)=0\,;\qquad(1)$$

$$\rho C_{p}u\cdot\nabla T=\nabla\cdot(\kappa\nabla T)+Q_{vh}\,;$$

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

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

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

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

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

- thermal insulation of upper matrix part:

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

- 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: $u = 0$,
- equality to zero of liquid velocity component perpendicular to the lateral side of the sample after leaving the matrix $u\ n = 0$,

where: u is velocity field, ρ is density, p is pressure, η is dynamic viscosity factor, κ is thermal conductivity, F is vector field of mass forces, Qvh is volumetric heat source due to internal friction, 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

The properties of thermoelectric material, which in simulation is considered to be a high-viscosity fluid, were determined experimentally, and their correlation was verified with the published data. For this model, it was necessary to determine the equivalent viscosity of the test fluid. The equivalent von Mises stresses can be found from the general deviator stress tensor [5] as

$$\sigma_{eqv}=\sqrt{\frac{3}{2}\tau:\tau}$$

or, using $\tau=2\eta\dot{\varepsilon}$, where $\dot{\varepsilon}$ is strain rate, η is velocity, as

$$\sigma_{eqv}=\sqrt{6\eta^2\varepsilon:\varepsilon}\ . \qquad (3.2)$$

Representing the equivalent strain rate as

$$\phi_{eqv}=\sqrt{\frac{3}{2}\varepsilon:\varepsilon}$$

the expression (3.2) can be re-written as

$$\sigma_{eqv}=3\eta\phi_{eqv}\,.$$

Strain rate tensor is determined as follows

$$\dot{\varepsilon} = \frac{\nabla u + (\nabla u)^T}{2} = \frac{1}{2}\dot{\gamma}\,.$$

Shear velocity:

$$\dot{\gamma} = |\dot{\gamma}| = \sqrt{\frac{1}{2}\dot{\gamma} : \dot{\gamma}}\,.$$

Accordingly,

$$\phi_{eqv} = \frac{1}{\sqrt{3}}\dot{\gamma}\,.$$

Flow rule

$$\sigma_{eqv} = \kappa_f$$

The flow rule specifies that plastic flow occurs when the equivalent stress σ_{eqv} reaches the flow stress, κf. Viscosity is defined as

$$\eta = \frac{\kappa_f}{3\phi_{eqv}}$$

The magnitude of the total flow stress is given by the expression for the generalized Zener-Hollomon function

$$\eta = \frac{asinh\left(\left(\frac{Z}{A}\right)^{1/n}\right)}{\sqrt{3}\alpha\dot{\gamma}}$$

where: $A = 2.39 * 10^8$ 1/s, $n = 2.976$, $\alpha = 0.052$ 1/MPa, $Z = \frac{1}{\sqrt{3}}\dot{\gamma}e^{\left(\frac{Q}{RT}\right)}$, Q=153kJ/mole, R=8.314 J/K*mole [5].

Fig. 2 shows a mesh of finite element method which is used in Comsol Multiphysics.

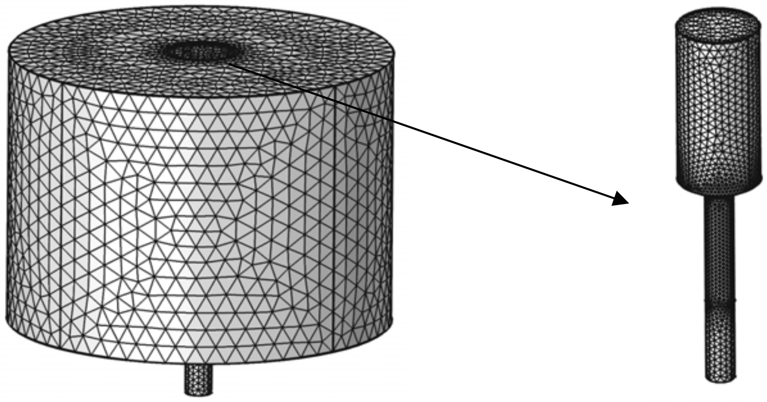
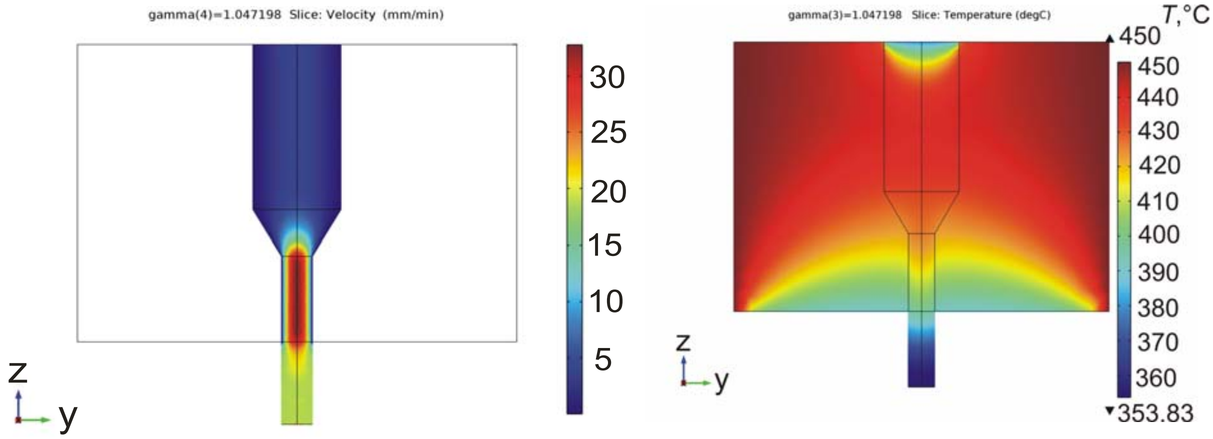


Fig. 2. Finite-element method mesh.

Computer simulation results

Velocity fields and temperature distributions in the matrix and thermoelectric material obtained by computer simulation for different matrix configurations (angles γ) are shown in Fig. 3-6. The velocity in mm/min and temperature in degrees Celsius are marked in colour.



a) *b)*

Fig. 3. Velocity field (a) of thermoelectric material inside the matrix and temperature distribution (b) in material and matrix (γ = 30°)

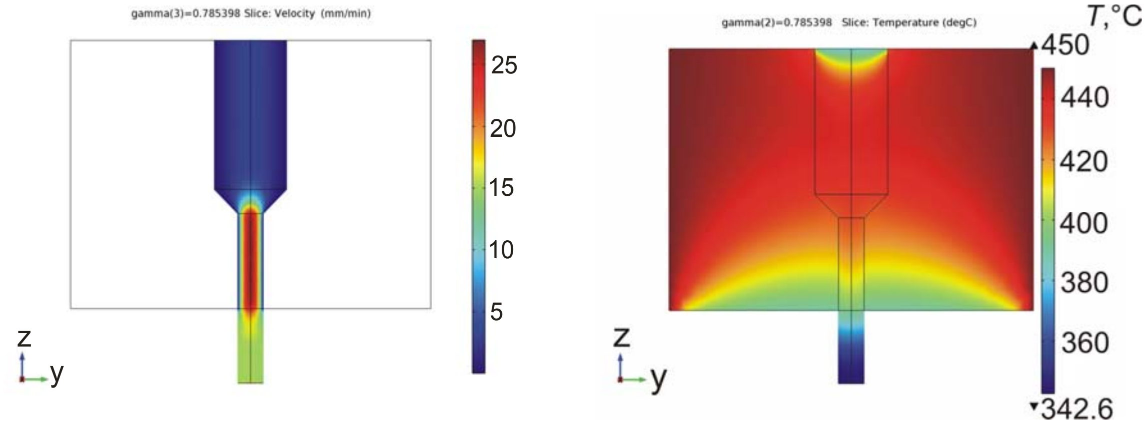


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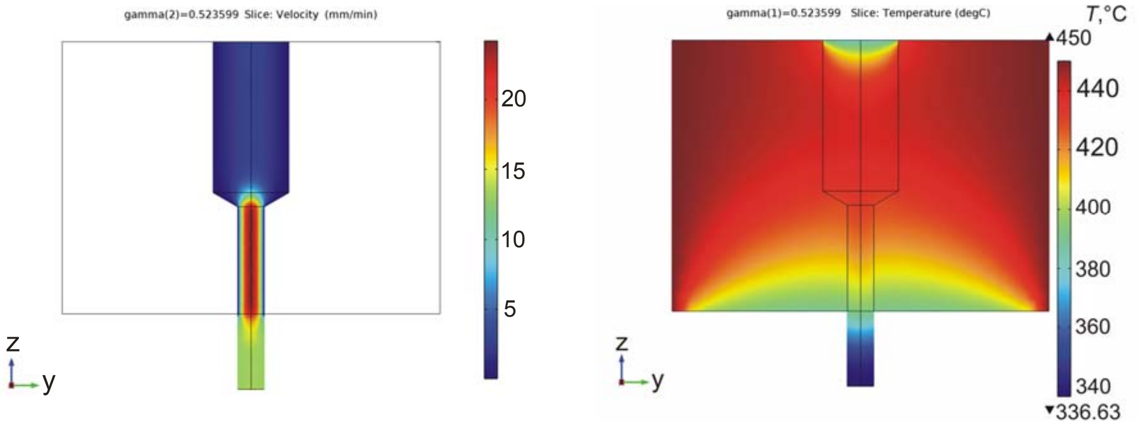
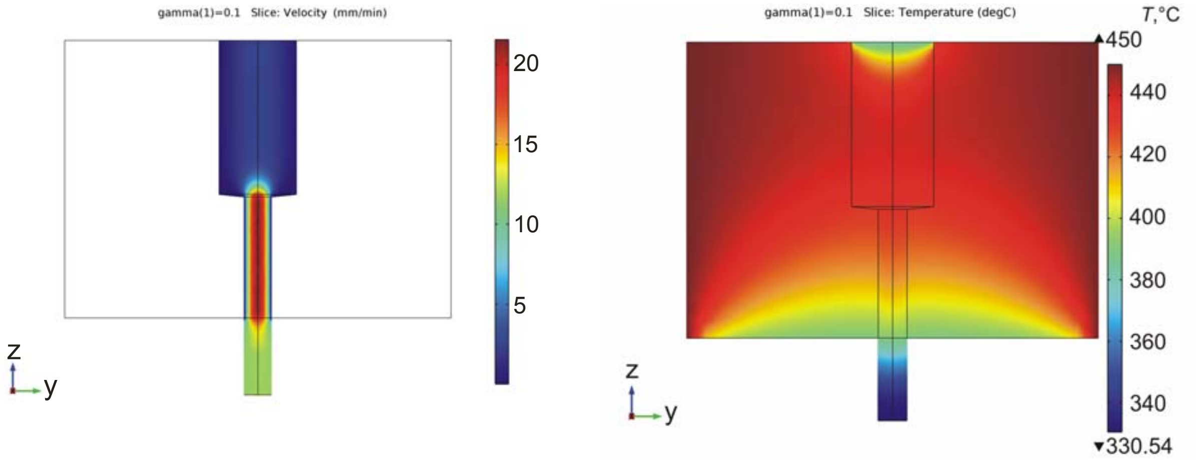
Fig. 4. Velocity field (a) of thermoelectric material inside the matrix and temperature distribution (b) in material and matrix (γ = 45°)



a) *b)*

Fig. 5. Velocity field (a) of thermoelectric material inside the matrix and temperature distribution (b) in material and matrix (γ = 60°)



a) *b)*

Fig. 6. Velocity field (a) of thermoelectric material inside the matrix and temperature distribution (b) in material and matrix (γ = 90°)

Matrix configuration for the case of three-stage extrusion is shown in Fig. 7.

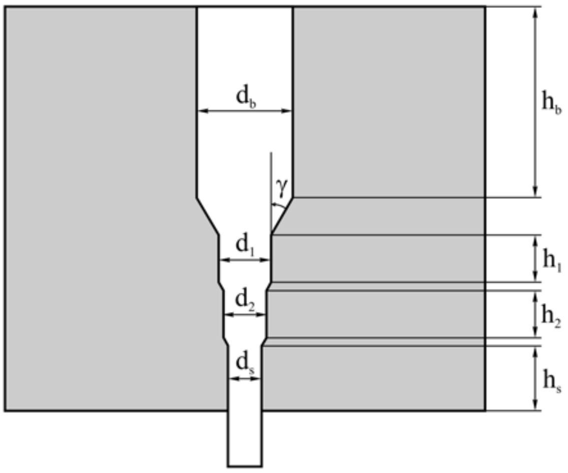
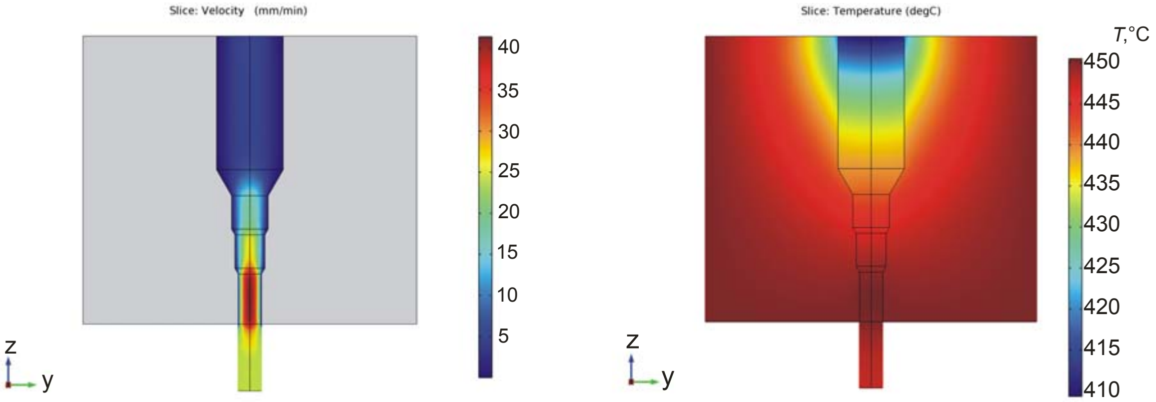


Fig. 7. Matrix for three-stage extrusion of thermoelectric material

Velocity field and temperature distribution for this case are shown in Fig.8.



a) *b)*

Fig. 8. Velocity field (a) of thermoelectric material inside the matrix and temperature distribution (b) in material and matrix for the case of three-stage extrusion

The developed computer model can serve the basis for optimizing the design of equipment for extrusion of Bi_2Te_3 based thermoelectric material in order to improve its efficiency and to enhance the quality of the material obtained.

Conclusions

1. A computer model of the hot extrusion process of Bi_2Te_3 based thermoelectric material has been created which can be used to study the distributions of temperature and material flow velocity in the matrix, as well as stress distribution in the matrix due to external pressure and thermal loads.
2. The temperature and velocity field distributions have been obtained depending on matrix configuration for the case of single-stage extrusion of Bi_2Te_3 based thermoelectric material.
3. The behavior of thermoelectric material in its passage through the matrix for the case of multistage extrusion of Bi_2Te_3 based thermoelectric material has been studied.

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НАБЛИЖЕННЯ В’ЯЗКОЇ РІДИНИ ПРИ МОДЕЛЮВАННІ ПРОЦЕСУ ЕКСТРУЗІЇ ТЕРМОЕЛЕКТРИЧНОГО МАТЕРІАЛУ НА ОСНОВІ Bi_2Te_3

У процесі екструзії заготовки матеріалу деформуються в практично ідеально пластичних умовах. Такий процес може бути змодельований з використанням теорії гідродинаміки, де матеріал розглядається як рідина з дуже високою в'язкістю, що залежить від швидкості й температури. Внутрішнє тертя шарів, що рухаються, матеріалу є також джерелом тепла, тому необхідно використовувати також рівняння переносу тепла в сукупності з гідродинамічною частиною задачі. Такий підхід є особливо ефективним для моделювання процесу екструзії термоелектричних матеріалів, коли присутні більші деформації. У даній роботі наведено результати об'єктно-орієнтованого комп'ютерного моделювання процесу гарячої екструзії термоелектричного матеріалу на основі Bi_2Te_3*. Розглянуто випадки одержання циліндричних зразків круглого перерізу для різних конфігурацій матриці у процесах одноступінчастої та багатоступінчастої екструзії. Отримані розподіли температури й швидкості течії матеріалу в матриці, а також розподіл напруг у матриці за рахунок зовнішнього тиску й теплових навантажень лягли в основу оптимізації устаткування для одержання екструдованого термоелектричного матеріалу. Бібл. 5, рис. 8, табл. 1.*

Ключові слова: екструзія, термоелектричний матеріал,моделювання

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ПРИБЛИЖЕНИЕ ВЯЗКОЙ ЖИДКОСТИ ПРИ МОДЕЛИРОВАНИИ ПРОЦЕССА ЭКСТРУЗИИ ТЕРМОЭЛЕКТРИЧЕСКОГО МАТЕРИАЛА НА ОСНОВЕ Bi_2Te_3

В процессе экструзии заготовки материала деформируются в практически идеальных пластических условиях. Такой процесс может быть смоделирован с использованием теории гидродинамики, где материал рассматривается как жидкость с очень высокой вязкостью, зависящей от скорости и температуры. Внутреннее трение движущихся слоев материала служит в качестве источника тепла, поэтому необходимо использовать также уравнения переноса тепла в совокупности с гидродинамической стороной задачи. Такой подход является особенно эффективным для моделирования процесса экструзии термоэлектрических материалов, когда присутствуют большие деформации. В настоящей работе приведены результаты объектно-ориентированного компьютерного моделирования процесса горячей экструзии термоэлектрического материала на основе Bi_2Te_3*. Рассмотрены случаи получения цилиндрических образцов круглого сечения для различных конфигурации матрицы при одноступенчатой и многоступенчатой экструзии. Получены распределения температуры и скорости течения материала в матрице, а также распределения напряжений в матрице за счет внешнего давления и тепловых нагрузок, которые легли в основу оптимизации оборудования для получения экструдированного термоэлектрического материала. Библ. 5, рис. 8, табл. 1.*

Ключевые слова: экструзия, термоэлектрический материал, моделирование.

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