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MODELING OF THE CRYSTALLIZATION PROCESS OF A POLYMER PLATE TAKING INTO ACCOUNT LARGE DEFORMATIONS

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The issues of modeling the thermomechanical behavior of a polymer material during cooling accompanied by crystallization are considered. The proposed approach is applied to the problem of deformation upon cooling of an infinite plate made of low-pressure polyethylene during crystallization. Mathematical formulations of thermal kinetic and thermomechanical boundary value problems are formulated. The results of the numerical solution of a coupled heat-kinetic problem, including the non-stationary heat conduction equation and the crystallization kinetics equation, are presented, provided that the characteristics of the material depend on temperature. When solving the boundary value problem of thermomechanics, the previously obtained phenomenological nonlinear constitutive relations are used, which continuously describe the behavior of a polymer material in a wide temperature range, including the range of phase transformations. The defining relations are obtained using the Peng – Landel potential. A weak variational statement of the boundary value problem, constructed using the Galerkin method, is presented. A linearization procedure is carried out, which makes it possible to reduce the solution of an initially nonlinear boundary value problem to solving a sequence of linear problems with relatively small increments of the displacement vector components. In this case, the linearization of geometric relations is performed by superimposing small increments of deformations on finite ones, linearization of the constitutive relations - expansion in a Taylor series with subsequent retention of linear terms under the assumption that the increment of the components of the strain tensor is small. An approach is demonstrated that naturally takes into account the small increments of temperature and structural deformations arising in the material. Aspects of the numerical implementation of the created algorithm based on the finite element technology of constructing a discrete analogue of the problem under consideration are analyzed. The results of solving the problem under discussion in a linear formulation under the assumption of small deformations and in a nonlinear formulation are presented and compared.

Key words: thermomechanics, polymers, crystallization, mathematic simulation, finite deformations, linearization, numerical approach

1. Introduction

Products made of polymeric materials are widely used in various industries. One of the stages in this production is the stage of forced cooling accompanied by the crystallization of the material. High technological stresses as a result of temperature and deformation inhomogeneities often lead to decreasing in the performance of products and even to their destruction at the manufacturing stage. In this regard, the problem of modeling thermomechanical processes in polymeric materials under conditions of phase transitions is of topical importance. The models of the behavior of such media should include constitutive relations that describe in a unified manner the relationship between the stress and strain tensors in a wide range of temperatures, including the temperatures of phase transformations. Due to the complexity in nature of real processes and the geometric variety of product shapes, the study of the patterns of forming technological stress fields is only possible by numerical methods. Therefore, it is of great importance to create a practical numerical algorithm for solving the thermomecanical boundary value problem of crystallizing polymer medium.

A large number of publications are devoted to the modeling of processes in curing polymer materials, [1–20] being only a few of them. A common feature of the models proposed in [1–3] is the aspiration to obtain the possibility of a simple estimate of residual stresses. Some authors, when constructing models of thermomechanical behavior, assume that the crystallizing polymer shows itself as an elastic material with small deformations. For example, in [4], with this assumption, the constitutive relations for amorphous-crystalline polymers were developed. In [5–12], the description of the polymer reaction to thermomechanical action was carried out within the framework of finite deformations. Many models are based on the elastic-viscoplastic approach [7–9, 13] and are intended either for specific polymer materials [5, 13], or are limited only by certain types of stress-strain state. For example, in [6] the model is aimed at representing the mechanical behavior of the polymer in the temperature range, including glass transition temperatures, for the cases of uniaxial

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loading and plane stress state. In [8], a coupled thermomechanical theory is proposed to simulate the dependence of the response of amorphous polymers on the strain rate and temperature under conditions of large strains.

At present, interest in the problems of describing the thermomechanical behavior of polymers during phase transformations is due to their widespread use in cases where shape memory is required in structural materials. In polymers, this effect is associated precisely with phase or relaxation transitions. The work [14] simulates the thermomechanical behavior of polymeric materials under conditions of relaxation transitions. The publications [11, 12, 15–20] are devoted to the studies of polymers response with shape memory effect to deformation effects. Thus, in [11, 12], a model of the behavior of a material is constructed, which undergoes a transition from a highly elastic state to a vitrified state and back during deformation and a concomitant change in temperature. The computation results are compared with experimental data.

It should be noted that the proposed models are often based on the hypothesis of small deformations and are intended to describe changes in the properties of polymer materials in a fairly narrow temperature range and with a specific mechanism for achieving the shape memory effect and cannot display other thermomechanical effects.

2. Modeling the thermomechanical behavior of a crystallizing plate

In order to illustrate the possibilities of the defining relations proposed by the authors earlier [21], formulated for conditions of finite deformations, in this work, we solved the model problem of deformation of an infinite plate of constant thickness made of low-pressure polyethylene under cooling. First, the material of the body under consideration was heated to a temperature exceeding the melting point. Further, the plate was cooled, and crystallization processes were being performed in the material accompanied by the heat release. It was required to investigate the evolution of the deformed state of the body from the effect of temperature and shrinkage deformations arising in the process of cooling and crystallization.

The problem was solved in two stages. At the first stage, the boundary value problem of unsteady thermal conductivity was solved paing attention to the crystallization of the material. At the second stage, on the basis of the data obtained on the evolution of the temperature fields and the degree of crystallization along the thickness of the platethe solution of the boundary value problem of crystallizing polymer was carried out. Since the process of deformation of the plate was accompanied by large temperature and shrinkage deformations, the problem was considered within the framework of the theory of finite deformations.

2.1. Thermal kinetic problem solution

The formulation of the problem within the framework of the well-known thermal kinetic model included:
– unsteady heat conduction equation

$$c(T)\rho(T)\frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left(\lambda(T)\frac{\partial T}{\partial x}\right)+\rho(T)Q_k\dot{\alpha}(t), \qquad x\in[0,L]; \tag{1}$$

– equation of kinetics of nonisothermal crystallization [22, 23]

$$\frac{d\alpha}{dt}=K\exp\left(-\frac{U}{RT}-\frac{\Psi}{T_m-T}\right)(1+A_0\alpha)\left(\alpha_e(T)-\alpha\right), \qquad x\in[0,L]; \tag{2}$$

– boundary and initial conditions

$$\frac{\partial T(0,t)}{\partial x}=0, \qquad \lambda\frac{\partial T(L,t)}{\partial x}=-h\big(T(L,t)-T_{am}(t)\big), \qquad (3)$$
$$T(x,0)=T_0, \qquad \alpha(x,0)=0, \qquad x\in[0,L].$$

In equations (1–3) the following notations were used: t - time; x - coordinate along the thickness of the plate; T - temperature; ρ - the density of the material; c - specific heat capacity; λ - coefficient of thermal conductivity; Q_k - the thermal effect of the crystallization reaction; α - the degree of crystallization of the material, which during the process changes from zero to a certain limiting value, depending on temperature and representing the equilibrium degree of crystallization α_e, $\dot{\alpha}=\partial\alpha/\partial t$; R - universal gas constant; K, U, ψ, A_0 - macrokinetic constants determined experimentally; h - heat transfer coefficient; T_m - melting temperature; T_{am} - ambient temperature; T_0 - initial temperature; L - half the thickness of the plate.

A numerical calculation was carried out for a plate made of low-pressure polyethylene. The values of its thermophysical and mechanical parameters were taken from the literature [24–26], the macrokinetic constants included in the equation of the kinetics of nonisothermal crystallization are given in Table 1.

When solving the thermal kinetic problem, the dependence of the specific heat capacity, thermal conductivity coefficient, density and equilibrium degree of polyethylene crystallization on temperature was taken into account (Table 2) [24, 25].

Table 1. Values of macrokinetic constants.

K, s^{-1}	U, J / mol	ψ, K	T_m, K	A_0	Q_k, J / kg
$2{,}33\cdot10^4$	30200	182	415	82	164000

Table 2. Values of thermophysical characteristics and equilibrium degree of crystallization depending on temperature.

T, K	c, J / (kg·K)	λ, W / (m·K)	ρ, kg / m^3	α_e
283	2250	0,228	947	0,9
341	2325	0,226	923	0,87
399	2395	0,182	832	0,41
457	2402	0,180	794	–

The temperature boundary value problem was solved numerically using the finite difference method. Due to symmetry, only half of the structure was considered. The plate thickness was assumed to be 20 mm, the initial body temperature was 450 K. Since the problem is of a model nature, taking into account the temperature dependence of the heat transfer coefficient is not of crucial importance for demonstrating the capabilities of the proposed approach. Therefore, the heat transfer coefficient was assumed to be constant, approximately corresponding to the case of a laminar infinite flow of water around a smooth plate at a speed of 0.5 m / s [27]. Its value was equal to 450 W / (m^2 K). The mesh used contained 100 coordinate nodes. The time step was 0.5 s. The counting process was terminated when the equilibrium degree of crystallization was reached at all points.

The solution of the kinetic equation of nonisothermal crystallization was found at each step of the algorithm for solving the boundary value problem and was determined numerically by the fourth-order Runge-Kutta method [28]. To ensure the stability of the counting, the time step was equal to 0.005 s.

Figure 1 shows the distribution curves of temperature and degree of crystallization for different points in time.

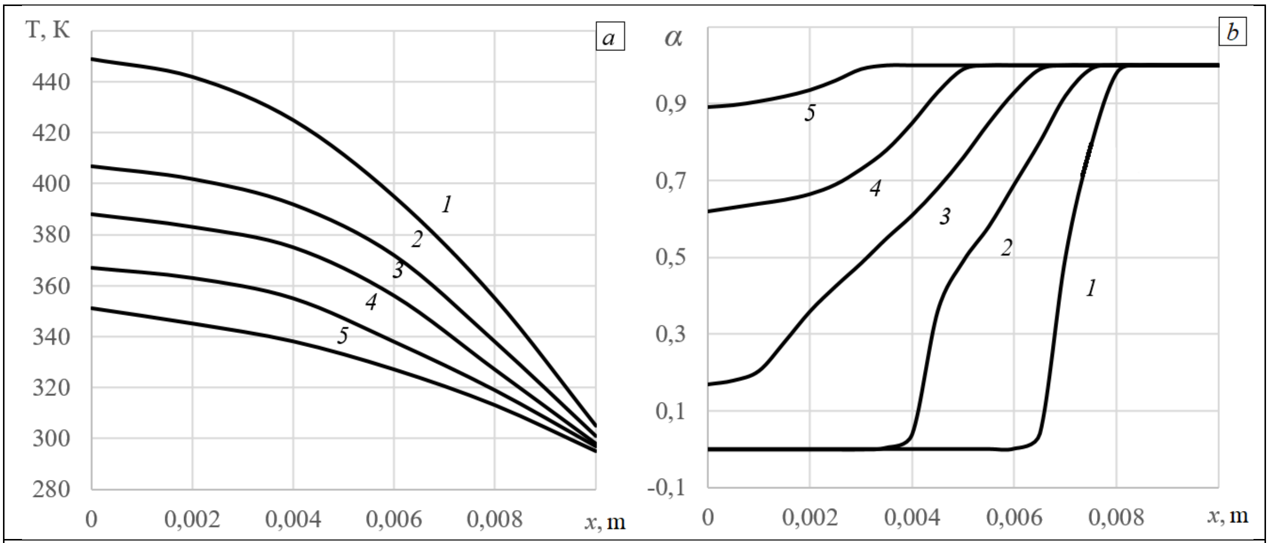

Fig. 1. Curves of temperature distribution (a) and degree of crystallization (b) over the plate thickness at different times, t s: 200 (curves 1), 400 (2), 600 (3), 800 (4), 1000 (5).

2.2. Solution of the boundary value problem of mechanics of crystallizing polymer

To solve the problem of mechanics, a "weak" variational statement was used, which for the discussed case has the form [29]:

$$\int_{V_0} \mathbf{P}_{II} \cdot\cdot\, \delta\mathbf{C}\, dV_0 = 0\,, \qquad (4)$$

where $\mathbf{P}_{II}$ is the Piola – Kirchhoff tensor of the second kind, $\mathbf{C}$ is the Cauchy – Green strain tensor, and V_0 is the initial volume of the body. The advantages of the variational formulation include the fact that it has been formulated in the initial configuration, which greatly simplifies the construction of numerical algorithms.

The relationship between the Piola – Kirchhoff tensor, which characterizes the stressed state of the material, with the elastic potential W was determined as

$$\mathbf{P}_{II} = 2\partial W\left(\mathbf{G}_t^{\times}\right) \big/ \partial \mathbf{G}_t^{\times}\,,$$

where $\mathbf{G}_{\mathbf{t}}^{\times}$ is the tensor of the Cauchy – Green strain measure at the current time moment t. The relationship between the tensor of the Cauchy – Green strain measure and the Cauchy – Green strain tensor was given by the expression $\mathbf{C} = \left(\mathbf{G}_t^{\times} - \mathbf{g}\right)\big/2$, where $\mathbf{g}$ is the metric tensor. The constitutive relations for an elastic crystallizing polymer material were taken in the form [29]:

$$W\left(\mathbf{G}_t^{\times}\right) = \left(1-\alpha(t)\right) W_a\left(\mathbf{G}_t^{\times}\right) + \int_0^{\alpha(t)} W_{cr}\left(\left(\mathbf{F}_\tau^{\mathrm{T}}\right)^{-1} \cdot \mathbf{G}_t^{\times} \cdot \mathbf{F}_\tau^{-1}\right) d\alpha(\tau)\,. \qquad (5)$$

In (5) $\mathbf{F}_\tau = \left(\overset{\tau}{\nabla}\mathfrak{R}\right)^{\mathrm{T}}$ is the place gradient tensor describing the transition from the configuration corresponding to the moment in time τ to the current configuration, $\overset{\tau}{\nabla}$ is the Hamilton operator defined with respect to the configuration corresponding to the moment in time τ, $\mathfrak{R}$ is the radius vector of the point in the current configuration, $\left(\mathbf{F}_\tau\right)^{-1}$, $\left(\mathbf{F}_\tau^{\mathrm{T}}\right)^{-1}$ are the inverse values of the gradient tensor the place $\mathbf{F}_\tau$ and the transposed tensor, W_a, W_{cr} are the elastic potentials of the amorphous and crystalline phases of the material.

Using the two-constant Peng – Landel potential [30] as the elastic potential, the expression for the relationship between the Piola – Kirchhoff tensor of the second kind $\mathbf{P}_{II}$ and the tensor of the Cauchy – Green strain measure was written as follows:

$$\mathbf{P}_{II}(t)=\left\{\mu^{a}\left[\left(I_3\left(\mathbf{G}_t^{\times}\right)\right)^{-1/3}\cdot\left(\mathbf{g}-\frac{I_1\left(\mathbf{G}_t^{\times}\right)}{3}\left(\mathbf{G}_{\tau t}^{\times}\right)^{-1}\right)\right]+B^{a}I_3\left(\mathbf{G}_t^{\times}\right)\left(\mathbf{g}-\left(I_3\left(\mathbf{G}_t^{\times}\right)\right)^{-1/2}\left(\mathbf{G}_t^{\times}\right)^{-1}\right)\right\}\left(1-\alpha(t)\right)+$$

$$+\int_0^{\alpha(t)}\left\{\mu^{cr}\left[\left(I_3\left(\mathbf{G}_{\tau t}^{\times}\right)\right)^{-1/3}\cdot\left(\mathbf{g}-\frac{I_1\left(\mathbf{G}_{\tau t}^{\times}\right)}{3}\left(\mathbf{G}_{\tau t}^{\times}\right)^{-1}\right)\right]+B^{cr}I_3\left(\mathbf{G}_{\tau t}^{\times}\right)\left(\mathbf{g}-\left(I_3\left(\mathbf{G}_{\tau t}^{\times}\right)\right)^{-1/2}\left(\mathbf{G}_{\tau t}^{\times}\right)^{-1}\right)\right\}d\alpha(\tau),\quad(6)$$

Where $\mathbf{G}_{\tau t}^{\times}=\left(\mathbf{F}_\tau^{\mathrm{T}}\right)^{-1}\cdot\mathbf{G}_t^{\times}\cdot\left(\mathbf{F}_\tau\right)^{-1}$, μ^{a}, B^{a}, μ^{cr}, B^{cr} are the mechanical characteristics of the amorphous and crystallized part of the material, respectively, I_1, I_3 are the first and third main invariants of the second-rank tensor, $\mathbf{g}$ is the metric tensor.

Formulation (4) is nonlinear, since it is based on nonlinear geometric and physical relationships. To create a numerical algorithm for determining the deformed state of a polymer plate under cooling, taking into account both the crystallization of its material and the resulting temperature and structural deformations, the initial problem formulation was linearized. This made it possible to reduce the procedure of obtaining a solution of the problem to the analysis of the sequence of solutions of linear elastic boundary value problems in the framework of the theory of small deformations. The presence of temperature and structural deformations of the material inherent in the processes under consideration is especially important in the mathematical formulation of physical relations in the case of using nonlinear equations of state. In [31], an approach is described, which is based on the procedure of linearization of physical relations under the assumption of a small value of temperature deformations at the considered transition.

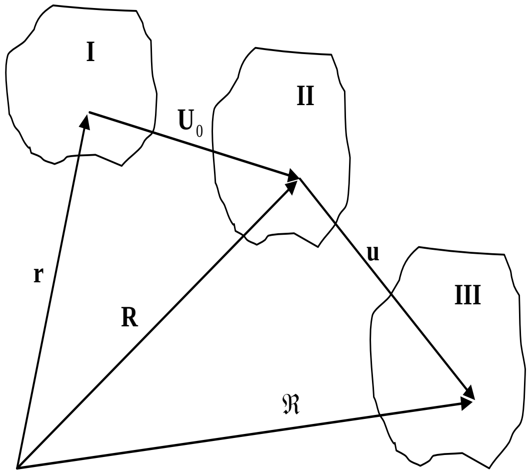

Fig. 2. Configurations sequentially acquired by the body in the process of deformation: I - initial, II - intermediate, III – final.

The construction of linearized geometric relationships is carried out as follows. First, the original movement of the body is decomposed into a set of small movements caused by small increments of external influences. According to the idea of superimposing small deformations on finite ones [32], the movement of a body from an initial configuration to a final one is represented as a superposition of its movements through intermediate configurations. In this case, the displacements of the points of the body at an arbitrary moment of time are recorded as the sum of their accumulated and small displacements during the transition from the intermediate configuration to the final one.

It is assumed that in the process of deformation, the body sequentially passes through three configurations (Fig. 2). The transition from the initial configuration to the intermediate one is determined by the displacement vector $\mathbf{U}_0$, and from the intermediate to the final one - by the vector of small displacements $\mathbf{u}$.

Taking into account the smallness of the displacements of the last transition $\mathbf{u}$, the Cauchy – Green tensor of elastic deformations, which describes the transition from the initial configuration to the final one, can be represented as a sum of two terms:

$$\mathbf{C} = \mathbf{C}_0 + \mathbf{F}_0^{\mathrm{T}} \cdot \mathbf{e}_E \cdot \mathbf{F}_0 \,. \tag{7}$$

Here: $\mathbf{C}_0$, $\mathbf{F}_0$ are tensor of elastic deformations and tensor gradient of place, describing the transition from the initial configuration to the intermediate one; $\mathbf{e}_E = \mathbf{e} - \mathbf{e}_\Theta$ is tensor of small elastic deformations arising at the transition from the intermediate configuration to the final one, and represented as the difference of total deformations $\mathbf{e} = \left[\overset{0}{\nabla}\mathbf{u} + \left(\overset{0}{\nabla}\mathbf{u} \right)^{\mathrm{T}} \right] \Big/ 2$ and deformations $\mathbf{e}_\Theta$, for the amorphous phase caused by temperature deformations, and for the crystalline phase - both temperature and structural deformations of the material at the considered transition; the Hamilton operator $\overset{0}{\nabla}$ is written with respect to an intermediate configuration. Thus, the obtained relations (7) began to linearly depend on the vector of small displacements $\mathbf{u}$, which determine the transition to the final configuration.

The procedure for linearizing the physical relations consisted in expanding expression (6) in a Taylor series taking into account the linear terms. Under the assumption of bounded deformations in the process under consideration, the linearized physical relations were written as follows

$$\mathbf{P}_{II}(t) = \left(\mathbf{P}_{II}\right)^0 + {}^4\mathbf{D}^a\left(\mathbf{C}_0\right) \cdot\cdot \left(\mathbf{F}_0^{\mathrm{T}} \cdot \left(\mathbf{e} - \mathbf{e}_\theta^a \right) \cdot \mathbf{F}_0 \right) \left(1 - \alpha(t) \right) + \int\limits_0^{\alpha(t)} {}^4\mathbf{D}^{\kappa p}\left(\mathbf{C}_{\tau 0}\right) \cdot\cdot \left(\mathbf{F}_0^{\mathrm{T}} \cdot \left(\mathbf{e} - \mathbf{e}_\theta^{cr} - \mathbf{e}_s^{cr} \right) \cdot \mathbf{F}_0 \right) d\alpha(\tau) \,. \tag{8}$$

Here: $\mathbf{e}_\theta^a$, $\mathbf{e}_\theta^{cr}$, $\mathbf{e}_s^{cr}$ - tensors describing the contribution of small temperature and structural deformations arising in the transition from an intermediate configuration to a final one: $\mathbf{e}_\theta^a = K_T^a \left(T(t) - T_0 \right) \mathbf{g}$, $\mathbf{e}_\theta^{cr} = K_T^{cr} \left(T(t) - T(\tau) \right) \mathbf{g}$, $\mathbf{e}_s^{cr} = k\mathbf{g}$; K_T^a, K_T^{cr} - coefficients of thermal expansion for amorphous and crystalline phases; k - coefficient of structural shrinkage; $\mathbf{C}_{\tau 0}$ - the tensor of the transition from the configuration corresponding to the time instant τ to the intermediate one; ${}^4\mathbf{D}^a$, ${}^4\mathbf{D}^{cr}$ are tensors of the fourth rank of the "tangential stiffness" of the amorphous and crystalline phases, the components of which depend on $\mathbf{C}_0$ and $\mathbf{C}_{\tau 0}$ and are determined as a result of linearization of relations (6).

As a result of the linearization procedures, the variational setting (4) was reduced to the form:

$$\begin{aligned} &\int\limits_{V_0} \Bigg[\left(\mathbf{P}_{II}\right)^0 + {}^4\mathbf{D}^a\left(\mathbf{C}_0\right) \cdot\cdot \left(\mathbf{F}_0^{\mathrm{T}} \cdot \left(\mathbf{e} - \mathbf{e}_\theta^a \right) \cdot \mathbf{F}_0 \right) \left(1 - \alpha(t) \right) \\ &+ \int\limits_0^{\alpha(t)} {}^4\mathbf{D}^{cr}\left(\mathbf{C}_{\tau 0}\right) \cdot\cdot \left(\mathbf{F}_0^{\mathrm{T}} \cdot \left(\mathbf{e} - \mathbf{e}_\theta^{cr} - \mathbf{e}_s \right) \cdot \mathbf{F}_0 \right) d\alpha(\tau) \Bigg] \cdot\cdot \delta\mathbf{C}^* dV_0 = 0, \end{aligned} \tag{9}$$

where $\mathbf{C}^* = \mathbf{F}_0^{\mathrm{T}} \cdot \mathbf{e} \cdot \mathbf{F}_0$.

Expression (9), formulated with respect to the increment of displacements arising from small increments of temperature and structural deformations, has become linear. Determination of the evolution of the displacement field was reduced to solving a sequence of linear problems with respect to increments of displacements at time steps.

Obtaining a solution to boundary value problems in mechanics for bodies of complex spatial configuration is impossible without the use of numerical techniques. Among the existing numerical approaches, the finite element method [33] is currently the most widely used, which was chosen to construct a discrete analogue of the problem under consideration. The finite element approach to the approximation of physical relations leads to linear algebraic relations, which in matrix form have the form:

$$\begin{gathered}\{P\}=\{P_0\}+\left[D^a(\mathbf{U}_0)\right]\left(\left[B(\mathbf{x},\mathbf{U}_0)\right]\{\delta^e\}-\{\Delta C_\theta^a\}\right)\left(1-\alpha(t)\right)\\+\int\limits_0^{\alpha(t)}\left[D^{cr}(\mathbf{U}_{0\tau})\right]\left(\left[B(\mathbf{x},\mathbf{U}_{0\tau})\right]\{\delta^e\}-\{\Delta C_\Theta^{cr}\}\right)d\alpha,\end{gathered}$$

where $\{\delta^e\}$ is the vector of nodal unknowns (increments of displacements at the current time step), $\left[B(\mathbf{x},\mathbf{U}_0)\right]$ is the matrix of element gradients, $\{\Delta C_\theta^a\}$ is the vector that takes into account the effect of increments of temperature deformations for the amorphous phase; $\{\Delta C_\Theta^{cr}\}$ is the vector, taking into account the influence of increments of temperature and structural deformations for the crystalline phase, $\left[D^a(\mathbf{U}_0)\right]$, $\left[D^{cr}(\mathbf{U}_{0\tau})\right]$ are matrices of "tangential" stiffness of the amorphous and crystalline phases of the material.

The last ratio can be converted to the form:

$$\{P\}=\{P_0\}+\left[D(\mathbf{U}_0)\right]\left[B(\mathbf{x},\mathbf{U}_0)\right]\{\delta^e\}-\left[D^a(\mathbf{U}_0)\right]\left(1-\alpha(t)\right)\{\Delta C_\theta^a\}-\int\limits_0^{\alpha(t)}\left[D^{cr}(\mathbf{U}_{0\tau})\right]\{\Delta C_\Theta^{cr}\}d\alpha\,,$$

where $\left[D(\mathbf{U}_0)\right]=\left[D^a(\mathbf{U}_0)\right]\left(1-\alpha(t)\right)+\int\limits_0^{\alpha(t)}\left[D^{cr}(\mathbf{U}_{0\tau})\right]d\alpha\,.$

Relation (9) can also be written in matrix form:

$$\sum_e\left([k]^e\delta^e-\{f_P\}^e-\{f_\Theta\}^e\right)=0\,,$$

where the symbol $\sum\limits_e$ means the summation over the elements, $[k]^e$ is the local stiffness matrix of the element, $\{f_P\}^e$ and $\{f_\Theta\}^e$ are the local vectors of the nodal forces caused by the accumulated stresses, thermal and structural deformations:

$$\begin{gathered}[k]^e=\int\limits_{V_0^e}\left[B(\mathbf{x},\mathbf{U}_0)\right]^{\mathrm{T}}\left[D(\mathbf{U}_0)\right]\left[B(\mathbf{x},\mathbf{U}_0)\right]dV\,,\\ \{f_P\}^e=\int\limits_{V_0^e}\left[B(\mathbf{x},\mathbf{U}_0)\right]^{\mathrm{T}}\{P_0\}dV\,,\\ \{f_\Theta\}^e=-\int\limits_{V_0^e}\left[B(\mathbf{x},\mathbf{U}_0)\right]^{\mathrm{T}}\left(\left[D^a(\mathbf{U}_0)\right]\left(1-\alpha(t)\right)\{\Delta C_\theta^a\}-\int\limits_0^{\alpha(t)}\left[D^{cr}(\mathbf{U}_{0\tau})\right]\{\Delta C_\Theta^{cr}\}d\alpha\right)dV\,.\end{gathered}$$

As a result of assembly for the entire ensemble of finite elements that form a mesh analogue of the computational domain, a global system is obtained:

$$\left[K(U_0)\right]\{u\}=\left\{F_p\right\}+\left\{F_\Theta\right\}, \tag{10}$$

where $\left[K(U_0)\right]$ is the global matrix of displacements of the system, which has symmetry and depends on the vector of accumulated displacements U_0; $\left\{F_p\right\}$, $\left\{F_\Theta\right\}$ - global vectors of "fictitious" efforts caused by the stresses accumulated to the current time step and the temperature and structural deformations arising at the considered transition.

Thus, the determination of the evolution of the deformed state of the plate under cooling, taking into account the crystallization of the material under conditions of large deformations, has been reduced to solving a sequence of linear problems (10) formulated with respect to increments of nodal displacements. In this case, the operator on the left side of (10) should be redefined at each time step. Changes in the components of the Cauchy strain tensor and the Piola – Kirchhoff tensor upon transition to the next configuration are found from relations (7) and (8). When calculating the displacements, it is convenient to take the time grid to coincide with the time grid of the temperature problem.

Table 3. Values of mechanical constants.

μ^a, Pa	B^a, Pa	μ^{cr}, Pa	B^{cr}, Pa
$4{,}19\cdot10^6$	$2{,}08\cdot10^8$	$5{,}93\cdot10^7$	$1{,}78\cdot10^8$

The values of the parameters of the mechanical model (6) used in the calculations are shown in Table 3. The following values of the coefficients of thermal expansion for the amorphous and crystalline phases and the coefficient of structural shrinkage of the material were taken [24, 34]: $K_T^a=2{,}8\cdot10^{-5}\,\text{K}^{-1}$, $K_T^{cr}=0{,}9\cdot10^{-5}\,\text{K}^{-1}$, $k=-0{,}1$. The finite element analogue contained 100 nodes. The time step was 0.5 s.

The distributions of displacements over the thickness of the plate at different times are shown in Figure 3. For comparison, curves are shown that correspond to the solution of a similar problem on the basis of linear physical and geometric relationships [22]. As can be seen from the graphs, with increasing time, the discrepancy between the results obtained for the nonlinear and linear formulations of the problem under consideration increases.

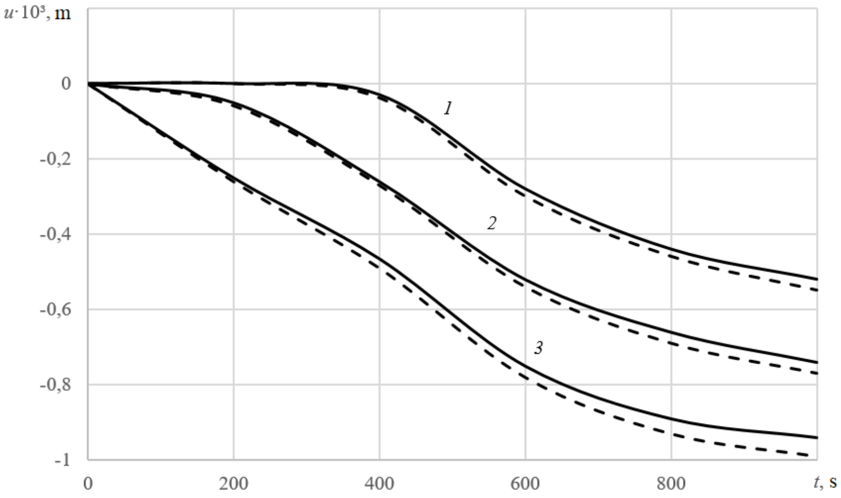

Fig. 3. Time dependences of displacements of characteristic points having different coordinates, m: 0.005 (curves 1), 0.0075 (2), 0.01 (3); solid lines correspond to the results obtained by the

nonlinear model, dashed lines - by the linear.

3. Conclusions

The proposed approach based on the procedure of linearization of the variational formulation of the thermomechanical boundary value problem of crystallizing medium made it possible to investigate the process of evolution of the deformed state in a cooled polymer plate under conditions of large deformations. The results obtained indicate that by the time the crystallization process is completed, the deformations in the plate reach 9.8%, which indicates the need to solve the problem under consideration within the framework of the theory of finite deformations. It was brought out that the data calculated by the nonlinear constitutive relations constructed by the authors earlier differ from those calculated within the framework of the linear model, while their discrepancy increases during the entire crystallization process.

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