QUASICONFORMAL MAPPING STUDY OF THE TEMPERATURE FIELD IN ANISOTROPIC FLEXIBLE-CHAIN POLYMERS

A.YA. BOMBA, V.V. KLEPKO[1], B.B. KOLUPAEV[2], E.V. LEBEDEV[1]

Rivne State Humanitarian University
(31, Ostafov Str., Rivne 33000, Ukraine),

[1]**Institute of Macromolecular Chemistry, Nat. Acad. Sci. of Ukraine**
(48, Kharkiv Rd., Kyiv 02160, Ukraine),

[2]**Taras Shevchenko Kyiv National University**
(6, Academician Glushkov Ave., Kyiv 03127, Ukraine)

UDC 519.57÷536.21

Temperature distribution in polyvinyl chloride (PVC) has been calculated and analyzed. The calculations were carried out using the method of conformal and quasiconformal mappings applied to anisotropic specimens confined by a thermal flow that is oriented with respect to the temperature gradient. A feedback effect of the thermal transfer on the medium characteristics has been taken into account. The results obtained are in good agreement with experimental data.

1. Introduction

Fabrication and study of polymer systems with the oriented structure are of significant scientific and practical interest [1]. Especially promising at that are the materials developed on the basis of polyvinyl chloride – a polymer, the manufacture of which in our country has been growing year by year [2]. The application of PVC as a heat-transfer or heat-insulating material has great potential. However, there is no completed theory for the determination of the temperature field and the thermal flow distribution in weakly anisotropic systems fabricated on the basis of linear flexible-chain polymers. The number of experimental researches, taking the complexity of their execution into account, is also confined [4]. All that demands the search for new simulation approaches and mathematical methods in order to consider and to analyze the processes of heat exchange in such polymer materials. Accordingly, this work aimed at studying the temperature field and the thermal flow distribution in weakly anisotropic PVC on the basis of the model proposed and using the method of conformal and quasiconformal mappings. Another purpose of the work was to specify the ways for a purposeful control of the thermal properties of composites.

2. Model

Consider PVC – a typical representative of linear flexible-chain polymers – in the framework of the Kirkwood–Riseman structural model [5] as a "pearl necklace": carbon skeleton atoms of the PVC chain look like "beads", the length of the arc segment is comparable with the contour length of the macromolecule, and the effective diameter of the latter is determined by the magnitude of the intermolecular coupling energy. In this case, supramolecular structure formations are realized in the form of either supergratings or microblocks with a limited lifetime τ [6]. It allows one to consider the PVC macromolecule as an "infinite crystal", which is formed by the condensed system of atoms [4]. Respectively, heat is transferred along both the main valence chain and the chain of intermolecular bonds. It has been demonstrated [7] that, if this system is considered as a number of structural subsystems, the equation of thermal balance holds true [2], because the mean free path of phonons at $T < T_g$ is restricted by linear dimensions of the body.

Consider heat conduction in a linear flexible-chain polymer, the anisotropic properties of which are induced by the orientation of macromolecular supergratings (microblocks) under the action of external forces [7]. For simplification, we suggest that the substance carriers of only a single kind are engaged into the energy exchange. Consider some portion ΔS of the macrosystem's area ($\Delta S \ll S$, where S is the specimen's area), which represents a structural subsystem. According to the energy conservation law, we will determine the specific energy flow transferred by thermal carriers and use the equation of thermal balance in the form of Fourier's relation, taking into account that the vector of the thermal flow density $\vec{v}$ is not parallel to the temperature gradient direction grad T. For this purpose, consider the distributions of the temperature and the thermal flow in a two-dimensional anisotropic polymer confined by four smooth curves. In accordance with work [8], we use a generalizing assumption that each component of the vector $\vec{\nu}$ at some point is a function of grad T at this point, i.e. that

$$\lambda_{11}\frac{\partial T}{\partial x}+\lambda_{12}\frac{\partial T}{\partial y}=\frac{\partial\psi}{\partial y};\quad \lambda_{21}\frac{\partial T}{\partial x}+\lambda_{22}\frac{\partial T}{\partial y}=-\frac{\partial\psi}{\partial x}, \tag{1}$$

where $\lambda=(\lambda_{ij})_{i,j=1,2}$ is the heat conductivity tensor and $\psi=\psi(x,y)$ is the function of thermal flow. That is, if $\psi(x,y)=\psi_1$ and $\psi(x,y)=\psi_2$ are two "outermost" flow lines, then the difference $\psi_1-\psi_2$ characterizes the thermal flow through the corresponding flow tube of the given specimen. The latter is the region $G_z=ABCD$ confined by the curves $AB=\{z=x+iy, f_1(x,y)=0\}$, $BC=\{z,f_2(x,y)=0\}$, $CD=\{z,f_3(x,y)=0\}$, and $DA=\{z,f_4(x,y)=0\}$. Solving system (1) by standard methods faces certain difficulties [7]. Therefore, in order to obtain a solution – in the region G_z – for the system of differential equations (1) which satisfies the boundary conditions

$$T|_{AB}=T_*\ ,\quad T|_{CD}=T^*\ ,\quad \psi|_{DA}=0\ ,\quad \psi|_{BC}=Q\ , \tag{2}$$

where Q is a total thermal flow to be find, we make the quasiconformal mapping $\omega=\omega(z)=T(x,y)+i\psi(x,y)$ of the region G_z onto the corresponding region of complex potential $G_\omega=\{\omega: T_*<T<T^*, 0<\psi<Q\}$. To ensure the smoothness of this mapping at nodal points $M=A$, B, C, and D, we demand that the functions $f_i(x,y)=0$ $(i=1\ldots4)$ obey the following conditions:

$$\Theta_M+\widetilde{\Theta}_M=\frac{\pi}{2}, \tag{3}$$

where

$$\cos\Theta_M=$$

$$=\frac{f'_{i-1_x}(M)\,f'_{i_x}(M)+f'_{i-1_y}(M)\,f'_{i_y}(M)}{\left(f'^2_{i-1_x}(M)+f'^2_{i-1_y}(M)\right)^{1/2}\left(f'^2_{i_x}(M)+f'^2_{i_y}(M)\right)^{1/2}},$$

$$\cos\tilde{\Theta}_M=\frac{\lambda_{11}f'^2_{j_x}(M)+(\lambda_{12}+\lambda_{21})\,f'_{j_x}(M)\,f'_{j_y}(M)+\lambda_{22}f'^2_{j_y}(M)}{\left(f'^2_{j_x}(M)+f'^2_{j_y}(M)\right)^{1/2}\left(\left(\lambda_{11}f'_{j_x}(M)+\lambda_{12}f'_{j_y}(M)\right)^2+\left(\lambda_{21}f'_{j_x}(M)+\lambda_{22}f'_{j_y}(M)\right)^2\right)^{1/2}}, \tag{4}$$

$$M=A,B,C,D,\quad f_0(M)\overset{df}{=}f_4(M),\, j=\begin{cases}1, & i=1,2,\\ 3, & i=3,4.\end{cases}$$

These conditions mean that the tangent to the heat flow line at each relevant point M must deviate from the normals to the equipotential lines by the same amount as the body's anisotropy deflects the vector of thermal flow velocity from them.

The corresponding analogs of orthogonality conditions in the vicinity of the boundary sections look like

$$-f_{k_x}'(x,y)\,y_\varphi+f'_{k_y}(x,y)\,x_\varphi=\left(f'^{\,2}_{k_x}(x,y)+f'^2_{k_y}(x,y)\right)^{1/2}\left(x^2_\varphi+y^2_\varphi\right)^{1/2}\left(1-\cos^2\Theta_k\right)^{1/2},\quad k=1,3, \tag{5}$$

$$\cos\Theta_k=\frac{\lambda_{11}f'^2_{k_x}(x,y)+(\lambda_{12}+\lambda_{21})\,f'_{k_x}(x,y)\,f'_{k_y}(x,y)+\lambda_{22}f'^2_{k_y}(x,y)}{\left(f'^2_{k_x}(x,y)+f'^2_{k_y}(x,y)\right)^{1/2}\left(\left(\lambda_{11}f'_{k_x}(x,y)+\lambda_{12}f'_{k_y}(x,y)\right)^2+\left(\lambda_{21}f'_{k_x}(x,y)+\lambda_{22}f'_{k_y}(x,y)\right)^2\right)^{1/2}},$$

$$f'_{l_x}(x,y)\,y_\psi-f'_{l_y}(x,y)\,x_\psi=\left(f'^2_{l_x}(x,y)+f'^2_{l_y}(x,y)\right)^{1/2}\left(x^2_{\psi\Psi}+y^2_\Psi\right)^{1/2}\left(1-\cos^2\Theta_l\right)^{1/2},\quad l=2,4, \tag{6}$$

$$\cos\Theta_l=\frac{\lambda_{11}f'^2_{l_x}(x,y)+(\lambda_{12}+\lambda_{21})\,f'_{l_x}(x,y)\,f'_{l_y}(x,y)+\lambda_{22}f'^2_{l_y}(x,y)}{\left(f'^2_{l_x}(x,y)+f'^2_{l_y}(x,y)\right)^{1/2}\left(\left(\lambda_{11}f'_{l_x}(x,y)+\lambda_{12}f'_{l_y}(x,y)\right)^2+\left(\lambda_{21}f'_{l_x}(x,y)+\lambda_{22}f'_{l_y}(x,y)\right)^2\right)^{1/2}}. \tag{7}$$

The cosine of the deflection angle of the velocity vector $\vec{\nu}$ from grad T at any interior point $z = x + iy$ is calculated by the formula

$$\cos\tilde{\Theta} = \\ = \frac{\lambda_{11} T_x'^2 + (\lambda_{12} + \lambda_{21}) T_x' T_y' + \lambda_{22} T_y'^2}{\sqrt{T_x'^2 + T_y'^2}\sqrt{\left(\lambda_{11} T_x' + \lambda_{12} T_y'\right)^2 + \left(\lambda_{21} T_x' + \lambda_{22} T_y'\right)^2}}.$$

In the case where $\lambda_{ij} = \lambda_{ij}(T, \psi)$ (a nonlinear direct problem), the inverse – with respect to Eqs. (2) and (2) – problem for a quasiconformal mapping $z = z(\omega) = x(T,\psi) + iy(T,\psi)$ of the region G_ω onto G_z one, provided that Q is unknown, looks like

$$\lambda_{11}(T,\psi)\frac{\partial y}{\partial \psi} - \lambda_{12}(T,\psi)\frac{\partial x}{\partial \psi} = \frac{\partial x}{\partial T},$$

$$\lambda_{21}(T,\psi)\frac{\partial y}{\partial \psi} - \lambda_{22}(T,\psi)\frac{\partial x}{\partial \psi} = \frac{\partial y}{\partial T}, \tag{8}$$

$$\begin{cases} f_1\left(x\left(T_*,\psi\right), y\left(T_*,\psi\right)\right) = 0, \\ f_2\left(x\left(T,Q\right), y\left(T,Q\right)\right) = 0, \\ f_3\left(x\left(T^*,\psi\right), y\left(T^*,\psi\right)\right) = 0, \ \ 0 \le \psi \le Q, \\ f_4\left(x\left(T,0\right), y\left(T,0\right)\right) = 0, \ \ T_* \le T \le T^*, \end{cases}$$

where $Q = \int_{AB} v_n dl$, and dl is an element of arc length. In this case, the corresponding equations of the second order for the functions $x = x(T,\psi)$ and $y = y(T,\psi)$ are

$$\begin{cases} \frac{\partial^2 x}{\partial T^2} + A(T,\psi)\frac{\partial^2 x}{\partial T \partial \psi} + B(T,\psi)\frac{\partial^2 x}{\partial \psi^2} + \\ +C(T,\psi)\frac{\partial x}{\partial T} + D(T,\psi)\frac{\partial x}{\partial \psi} = 0, \\ \frac{\partial^2 y}{\partial T^2} + A(T,\psi)\frac{\partial^2 y}{\partial T \partial \psi} + B(T,\psi)\frac{\partial^2 y}{\partial \psi^2} + \\ +E(T,\psi)\frac{\partial y}{\partial T} + F(T,\psi)\frac{\partial y}{\partial \psi} = 0, \end{cases} \tag{9}$$

where

$$A = \lambda_{12} - \lambda_{21}, \quad B = \lambda_{11}\lambda_{22} - \lambda_{21}\lambda_{12},$$

$$C = \frac{\lambda_{11_\psi}\lambda_{21} - \lambda_{11_T}\lambda_{21_T}}{\lambda_{11}} - \lambda_{21_\psi},$$

$$D = \lambda_{22_\psi}\lambda_{11} + \lambda_{12_T}\lambda_{21} - \lambda_{21_\psi}\lambda_{12} - \lambda_{12_\psi}\lambda_{21} + \\ + \frac{\lambda_{11_\psi}\lambda_{21}\lambda_{12} - \lambda_{12}\lambda_{11_T}\lambda_{21_T}}{\lambda_{11}},$$

$$E = \lambda_{12_\psi} - \frac{\lambda_{22\psi}\lambda_{12} + \lambda_{22_T}\lambda_{12_T}}{\lambda_{22}},$$

$$F = \lambda_{11_\psi}\lambda_{22} - \lambda_{21_T}\lambda_{12} - \lambda_{21_\psi}\lambda_{12} - \lambda_{12_\psi}\lambda_{21} + \\ + \frac{\lambda_{22_\psi}\lambda_{21}\lambda_{12} + \lambda_{21}\lambda_{22_T}\lambda_{12_T}}{\lambda_{22}}.$$

The application of such an approach allows one to pass from solving the direct problems to dealing with the problems of quasiconformal mappings of the corresponding regions of the quasicomplex potential onto initial (physical) ones. It also enables one to take into account the unknown parameters (the thermal flow) and the extra conditions that are imposed onto the solutions [8].

In accordance with work [8], we write down the finite-difference analogs of the equations in the region G_ω^γ in the form

$$\begin{cases} x_{i+1,j} + x_{i-1,j} - 2\left(1+\gamma^2 B_{i,j}\right)x_{i,j} + \gamma^2 B_{i,j}\left(x_{i,j-1} + x_{i,j+1}\right) + \frac{\gamma}{4}A_{i,j}\left(x_{i+1,j+1} + x_{i-1,j-1} - \right. \\ \left. -x_{i+1,j-1} - x_{i-1,j+1}\right) + \frac{\Delta T}{2}\left(\gamma D_{i,j}\left(x_{i,j+1} - x_{i,j-1}\right) + C_{i,j}\left(x_{i+1,j} - x_{i-1,j}\right)\right) = 0, \\ y_{i+1,j} + y_{i-1,j} - 2\left(1+\gamma^2 B_{i,j}\right)y_{i,j} + \gamma^2 B_{i,j}\left(y_{i,j-1} + y_{i,j+1}\right) + \frac{\gamma}{4}A_{i,j}\left(y_{i+1,j+1} + y_{i-1,j-1} - \right. \\ \left. -y_{i+1,j-1} - y_{i-1,j+1}\right) + \frac{\Delta T}{2}\left(\gamma F_{i,j}\left(y_{i,j+1} - y_{i,j-1}\right) + E_{i,j}\left(y_{i+1,j} - y_{i-1,j}\right)\right) = 0; \quad i = \overline{1,m}, \quad j = \overline{1,n}, \end{cases} \tag{10}$$

$$\begin{cases} f_1\left(x_{0,j}, y_{0,j}\right) = 0, & f_3\left(x_{m+1,j}, y_{m+1,j}\right) = 0, & j = \overline{0, n+1}, \\ f_2\left(x_{i,n+1}, y_{i,n+1}\right) = 0, & f_4\left(x_{i,0}, y_{i,0}\right) = 0, & i = \overline{0, m+1}, \end{cases} \tag{11}$$

$$-f'_{1_x}\left(x_{0,j}, y_{0,j}\right)\left(y_{1,j} - y_{0,j}\right) + \\ + f'_{1_y}\left(x_{0,j}, y_{0,j}\right)\left(x_{1,j} - x_{0,j}\right) =$$

$$= \left(f'^2_{1_x}\left(x_{0,j}, y_{0,j}\right) + f'^2_{1_y}\left(x_{0,j}, y_{0,j}\right)\right)^{1/2}\left(\left(x_{1,j} - x_{0,j}\right)^2 + \right. \\ \left. + \left(y_{1,j} - y_{0,j}\right)^2\right)^{1/2}\left(1 - \cos^2\Theta_{1_{0,j}}\right)^{1/2},$$

$$-f'_{3_x}(x_{m+1,j},y_{m+1,j})(y_{m,j}-y_{m+1,j})+$$

$$+f'_{3_y}(x_{m+1,j},y_{m+1,j})(x_{m,j}-x_{m+1,j})=$$

$$=\left(f'^2_{3_x}(x_{m+1,j},y_{m+1,j})+f'^2_{3_y}(x_{m+1,j},y_{m+1,j})\right)^{1/2}\times$$

$$\times\left((x_{m+1,j}-x_{m,j})^2+(y_{m+1,j}-y_{m,j})^2\right)^{1/2}\times$$

$$\times\left(1-\cos^2\Theta_{3_{m+1,j}}\right)^{1/2},$$

$$f'_{2_x}(x_{i,n+1},y_{i,n+1})(y_{i,n}-y_{i,n+1})-$$

$$-f'_{2_y}(x_{i,n+1},y_{i,n+1})(x_{i,n}-x_{i,n+1})=$$

$$=\left(f'^2_{2_x}(x_{i,n+1},y_{i,n+1})+f'^2_{2_y}(x_{i,n+1},y_{i,n+1})\right)^{1/2}\times$$

$$\times\left((x_{i,n+1}-x_{i,n+1})^2+(y_{i,n}-y_{i,n+1})^2\right)^{1/2}\times$$

$$\times\left(1-\cos^2\Theta_{2_{i,n+1}}\right)^{1/2},$$

$$f'_{4_x}(x_{i,0},y_{i,0})(y_{i,1}-y_{i,0})-f'_{4_y}(x_{i,0},y_{i,0})(x_{i,1}-x_{i,0})=$$

$$=\left(f'^2_{4_x}(x_{i,0},y_{i,0})+f'^2_{4_y}(x_{i,0},y_{i,0})\right)^{1/2}\times$$

$$\times\left((x_{i,1}-x_{i,0})^2+(y_{i,1}-y_{i,0})^2\right)^{1/2}\left(1-\cos^2\Theta_{4_{i,0}}\right)^{1/2},$$

$$i=\overline{0,m+1},\quad j=\overline{0,n+1}, \tag{12}$$

$$\gamma=\frac{1}{(m+1)(n+1)}\sum_{i,j=0}^{m,n}\left\{\left((x_{i+1,j}-x_{i,j})^2+\right.\right.$$

$$\left.+(y_{i+1,j}-y_{i,j})^2\right)^{1/2}+\left((x_{i+1,j+1}-x_{i,j+1})^2+\right.$$

$$\left.\left.+(y_{i+1,j+1}-y_{i,j+1})^2\right)^{1/2}\right\}/(a_1+a_2),$$

$$a_1=\left((\lambda_{11}(y_{i,j+1}-y_{i,j})-\lambda_{12}(x_{i,j+1}-x_{i,j}))^2+\right.$$

$$\left.+(\lambda_{21}(y_{i,j+1}-y_{i,j})-\lambda_{22}(x_{i,j+1}-x_{i,j}))^2\right)^{1/2},$$

$$a_2=\left(\left(\lambda_{11}(y_{i+1,j+1}-y_{i+1,j})-\right.\right.$$

$$\left.-\lambda_{12}(x_{i+1,j+1}-x_{i+1,j})\right)^2+(\lambda_{21}(y_{i+1,j+1}-y_{i+1,j})-$$

$$\left.-\lambda_{22}(x_{i+1,j+1}-x_{i+1,j}))^2\right)^{1/2}, \tag{13}$$

where $A_{i,j}=A(T_i,\psi_j)$, $B_{i,j}=B(T_i,\psi_j)$, $C_{i,j}=C(T_i,\psi_j)$, $D_{i,j}=D(T_i,\psi_j)$, $E_{i,j}=E(T_i,\psi_j)$, and $F_{i,j}=F(T_i,\psi_j)$.

If $\lambda_{ij}=\lambda_{ij}(x,t)$, the inverse problem is essentially nonlinear, and the equations for $x=x(T,\psi)$ and $y=y(T,\psi)$ look like

$$\begin{cases}\dfrac{\partial}{\partial\psi}\left(\dfrac{\lambda_{11}(x,y)\lambda_{22}(x,y)-\lambda_{21}(x,y)\lambda_{12}(x,y)}{\lambda_{11}(x,y)}\dfrac{\partial x}{\partial\psi}-\dfrac{\lambda_{21}(x,y)}{\lambda_{11}(x,y)}\dfrac{\partial x}{\partial T}\right)+\dfrac{\partial}{\partial\varphi}\left(\dfrac{1}{\lambda_{11}(x,y)}\dfrac{\partial x}{\partial T}+\dfrac{\lambda_{12}(x,y)}{\lambda_{11}(x,y)}\dfrac{\partial x}{\partial\psi}\right)=0,\\[2ex] \dfrac{\partial}{\partial\psi}\left(\dfrac{\lambda_{11}(x,y)\lambda_{22}(x,y)-\lambda_{21}(x,y)\lambda_{12}(x,y)}{\lambda_{22}(x,y)}\dfrac{\partial y}{\partial\psi}+\dfrac{\lambda_{12}(x,y)}{\lambda_{22}(x,y)}\dfrac{\partial y}{\partial T}\right)+\dfrac{\partial}{\partial\varphi}\left(\dfrac{1}{\lambda_{22}(x,y)}\dfrac{\partial y}{\partial T}-\dfrac{\lambda_{21}(x,y)}{\lambda_{22}(x,y)}\dfrac{\partial y}{\partial\psi}\right)=0,\end{cases} \tag{14}$$

The corresponding finite-difference analogs can be written down similarly to Eqs. (10)–(13). In accordance with work [8], the algorithm for finding the approximate solution of the problem is built for the finite-difference analogs of Eqs. (9) and (14), the definite boundary conditions, and the conditions of orthogonality and quasiconformal similarity in the small volumes of the corresponding grid parallelograms:

$$G_{\omega}^{\gamma}=\left\{\begin{array}{l}(T_i;\psi_j)\,;\;T_i=T_*+\Delta T_i,\quad i=\overline{0,m+1};\psi_j=\Delta\psi_j,\quad j=\overline{0,n+1};\\ \Delta T=\dfrac{T^*-T_*}{m+1};\;\;\Delta\psi=\dfrac{Q}{n+1};\;\;\gamma=\dfrac{\Delta T}{\Delta\psi};\;m,n\in N\end{array}\right\}. \tag{15}$$

3. Experiment, Results, and Their Discussion

For our researches, we used C-65$^{\mathrm{TM}}$ PVC with a molecular weight of 1.4×10^5. Specimens were prepared in the $T-p$ regime at $T=393$ K and $p=10.0$ MPa. The temperature dependence of the PVC heat conductivity λ was measured on modified IT-λ-400 and 3427-1000 °C installations [9] at a specimen heating rate of 3 °C/ min.

The capabilities of a λ-calorimeter were used to determine the distributions of the temperature and the thermal flow in PVC following the technique described in work [7]. The calculations of corresponding quantities were carried out according to expressions (9) and (14). The calculation procedure was as follows. The two-dimensional PVC system was divided into $m+1$ intervals along the direction of grad T and into $n+1$ intervals along the perpendicular direction $\psi(x,y)$. Without loss of generality, let the step along each direction be equal to unity. Consider a nodal point (i,j) of the grid ($0\le i\le m+1, 0\le j\le n+1$), the temperature of which changes in time t (we suppose that $t\ll\tau$). The distribution of the temperature T in a subsystem ΔS is a function of spatial coordinates (x and y in the two-dimensional problem) and surrounding temperatures. To simplify the calculations, we adopted that the linear approximation and identical distributions of T and ψ (see Eqs. (9), (11), and (14)) are valid for all subsystems. The functions that determine the position and the temperature of a boundary point will be designated as X_m^{nj}, T_i^{nj} and Y_i^{nj}, T_m^{nj}, respectively.

If the displacement of a boundary nodal point along the normal $\bar{n}$ for the time t is equal to $\Delta n=t\upsilon$, where υ is the specimen heating rate, the corresponding displacements along the x and y axes are

$$\Delta x=\frac{\Delta n}{\cos(\Delta\bar{n},\bar{x})}=\frac{\upsilon t}{\cos(\bar{n},\bar{x})},$$

$$\Delta y=\frac{\upsilon t}{\cos(\bar{n},\bar{y})},$$

respectively, where $(\bar{n},\bar{x})$ and $(\bar{n},\bar{y})$ are the angles between the normal $\bar{n}$ and the x or y axis, respectively; those angles satisfy the relations $0<(\bar{n},\bar{x})<\frac{\pi}{2}$, $0<(\bar{n},\bar{y})<\frac{\pi}{2}$, and $(\bar{n},\bar{x})+(\bar{n},\bar{y})=\frac{\pi}{2}$.

According to the algorithm described in work [8], we find the temperature distribution over the region ΔS of the specimen and the magnitude of the thermal flow through its arc element dl. This enables us to determine the temperature dependence of the effective value λ of PVC by the formula $\lambda=\left(\int_{(\ l)}\nu_n dl\right)/\Delta T$ and to compare the results obtained with experimental data (see Table).

Note that a homogeneous anisotropic medium can be simulated, e.g., as follows. Some point of the specimen's plane serves as an origin for an equidistant radial grid of rays. On each ray and at the same distance from the center, we cut off specimens of identical dimensions and shapes, place them into a λ-calorimeter, and determine the value of λ_{id} for each of them. From the set of results obtained, we select those with maximal or minimal heat conductivity and use them to determine the directions of specimen orientation. In the course of specimen heating, we correlate the quantity $\lambda_{\mathrm{id}}=\lambda_{\mathrm{id0}}+\varepsilon|\mathrm{grad}\ T|$. For the next time step, we fix the parameters of the medium and recalculate the temperature field again. Such a "by turn" fixation of the medium characteristics or the process is

Temperature dependence of the PVC heat conductivity λ

T K	λ_{exp}, 10^2 J·s^{-1}·m^{-1}·K^{-1}	λ_{cal}, 10^2 J·s^{-1}·m^{-1}·K^{-1}
273	14.8	14.6
283	15.0	14.9
293	15.6	15.3
303	16.3	16.1
313	16.7	16.5
323	17.0	16.9
333	17.5	17.2
343	18.0	17.8
353	18.3	18.1
363	18.6	18.5
373	18.7	18.8

carried out till their stabilization. Note that, despite the stationary formulation of the problem, the potential steps described above can be regarded as those corresponding to the development of the process in time from the beginning to the stabilization.

The examined method allowed the function $\lambda = f(T)$ to be approximated by the empirical formula $\lambda = \lambda_0 + \alpha [f(T)] = \lambda_0 + AT + BT^2$, where $\lambda_0 = 0.148$ W/(m × K), $A = 1.36 \times 10^{-4}$, and $B = -0.2 \times 10^{-6}$.

4. Conclusions

The method proposed enabled the temperature dependence of the effective heat conductivity λ of linear flexible-chain polymers to be calculated and studied. It has been demonstrated that, by varying the parameters λ_{12}, λ_{21}, λ_{11}, and λ_{22} (it can be done by introducing fillers or applying external fields), one can purposefully control the thermal properties of the system.

1. L.N. Novichenok and Z.P. Shulman, *Thermal Properties of Polymers* (Nauka i Tekhnika, Minsk, 1971) (in Russian).
2. S.Ya. Frenkel, *Macromolecule* in *Encyclopedia of Polymers* (Sovetskaya Entsyklopediya, Moscow, 1974), Vol. 2 (in Russian).
3. A.I. Slutsker, *Anisotropy of Polymer Properties* in *Encyclopedia of Polymers, Vol. 1* (Sovetskaya Entsyklopediya, Moscow, 1972) (in Russian).
4. Yu.Ya. Gotlib, V.G. Baranov, and A.V. Maksimov, Vysokomol. Soedin. A **29**, 2620 (1987).
5. A.L. Volynskii and N.F. Bakeev, Vysokomol. Soedin. C **47**, 1332 (2005).
6. S.Ya. Frenkel, I.M. Tsygelnyi, and B.S. Kolupaev, *Molecular Cybernetics* (Svit, Lviv, 1990) (in Russian).
7. A.V. Lykov, *Analytical Heat Diffusion Theory* (Academic Press, New York, 1968).
8. A.Ya. Bomba and C.C. Kashtan, Volynsk. Matemat. Visn. N 6, 3 (1999).
9. B.S. Kolupaev, in *Relaxation and Thermal Properties of Filled Polymer Systems*, edited by S.Ya. Frenkel (Vyshcha Shkola, Lviv, 1980) (in Russian).

Received 10.01.06.
Translated from Ukrainian by O.I.Voitenko

ДОСЛІДЖЕННЯ ТЕМПЕРАТУРНОГО ПОЛЯ В АНІЗОТРОПНИХ ГНУЧКОЛАНЦЮГОВИХ ПОЛІМЕРАХ МЕТОДОМ КВАЗІКОНФОРМНИХ ВІДОБРАЖЕНЬ

А.Я. Бомба, В.В. Клепко, Б.Б. Колупаев, Є.В. Лебедев

Р е з ю м е

Методом конформних і квазіконформних відображень в анізотропних зразках, обмежених тепловим потоком, орієнтованим відносно градієнта температури, розраховано і проаналізовано розподіл температурного поля в полівінілхлориді (ПВХ). Враховано зворотний вплив теплового переносу на характеристики середовища. Отримані результати добре узгоджуються з даними експерименту.