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MATERIALS SCIENCE

METHODOLOGY OF DIGITAL PREDICTION OF DEFORMATION PROCESSES OF POLYMER TEXTILE MATERIALS

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Prediction of deformation processes of polymer textile materials traditionally encounters objective difficulties caused by the heterogeneity in the rheological structure of such materials. The broad use of polymer textile materials in various technology sectors, from household polymers to space rocket coatings and deep-water apparatuses, makes it necessary to develop modern methods for predicting with increased accuracy their functional properties, including various deformation processes. The development of new digital methods for predicting deformation processes of polymer textile materials is based on the need to design new innovative items based on these materials with the required functionality and improved competitiveness.

The main purpose of predicting the deformation processes of polymer textile materials is to determine their functionality. Therefore, the more accurate the prediction is, the more reliable the information about the functional properties of such materials will be.

The deformation processes of polymer textile materials are traditionally predicted based on classical integral relationships of the Boltzmann–Volterra nonlinear-hereditary type with various integral cores [1].

The main objective difficulties encountered with this prediction concern the integral cores, ideally suitable for predicting deformation processes of polymer textile materials of a single macrostructure and certain component composition and entirely unsuitable for predicting operating processes of polymer materials of a different macrostructure or other component composition. Therefore, a sampling experiment is the main reliability and accuracy criterion of this prediction of deformation processes [2].

The main deformation processes of polymer textile materials determining their functionality are relaxation and creep. Classical methods of predicting these processes are based on numerical solution of Boltzmann–Volterra integral equations with various integral cores [3].

The defining Boltzmann–Volterra equation for predicting a relaxation process is a time-dependent process of changing stress in a polymer material because of a deformation applied to the material and is written [4]:

$$\sigma_t = E_0 \cdot \varepsilon_t - (E_0 - E_\infty) \cdot \int_0^t \varepsilon_{t-s} \cdot \frac{\partial \varphi_{\varepsilon s}}{\partial s} \cdot ds \ , \qquad (1)$$

where ε_t is a deformation changing with time t; σ_t, a stress changing with time t; E_0, elasticity modulus; E_∞, viscoelastic modulus; $\varphi_{\varepsilon t} \in (0;1)$, a relaxation function forming the basis of the relaxation integral core $\partial\varphi_{\varepsilon t}/\partial t$.

By analogy, the defining Boltzmann–Volterra equation for predicting creep is a time-dependent process of the change of deformation of the polymer material because of the stress applied to it and is written [5]:

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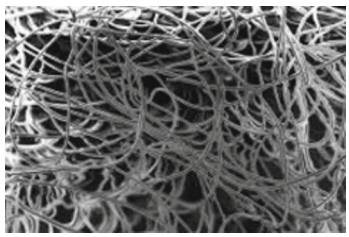

Fig. 1.

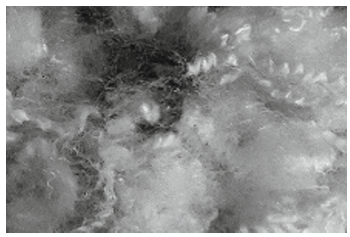

Fig. 2.

Fig. 1. Photograph of textile yarn prepared from polyester fiber.

Fig. 2. Photograph of polyester fiber raw material for preparing polyester textile yarn.

$$\varepsilon_t = \frac{1}{E_0} \cdot \sigma_t + \left(\frac{1}{E_\infty} - \frac{1}{E_0} \right) \cdot \int_0^t \sigma_{t-s} \cdot \frac{\partial \varphi_{\sigma s}}{\partial s} \cdot ds \ , \tag{2}$$

where $\varphi_{\sigma t} \in (0;1)$ is a creep function (creep) forming the basis of the creep integral core $\partial\varphi_{\sigma t}/\partial t$.

The scientific direction for mathematical modeling, systemic analysis, and computational prediction of deformation–relaxation functional properties of polymer materials developed by us presupposes the use of normalized functions as relaxation and creep functions [6].

The existence of several different relaxation and creep functions is justified because predictions of deformation processes that are independent of each other can be obtained.

Predicted deformation characteristics obtained by averaging characteristics determined using various mathematical models have a higher degree of reliability than those determined using a single mathematical model [7].

Simple relaxation in which the deformation of a polymer material remains constant (ε = const) is a special case of a relaxation process. Equation 1 is simplified for simple relaxation [8]:

$$\sigma_t = E_0\varepsilon - (E_0 - E_\infty)\varepsilon\varphi_{\varepsilon t} \tag{3}$$

or

$$\sigma_t/\varepsilon = E_{\varepsilon t} - (E_0 - E_\infty)\varphi_{\varepsilon t}, \tag{4}$$

where $E_{\varepsilon t}$ is the relaxation modulus of the polymer material.

Simple creep in which the stress applied to a polymer material remains constant (σ = const) is a special case of the creep process. Equation 2 is simplified for simple creep:

$$\varepsilon_t = \frac{1}{E_0} \cdot \sigma + \left(\frac{1}{E_\infty} - \frac{1}{E_0} \right) \sigma\varphi_{\sigma t} \tag{5}$$

or

$$\frac{\varepsilon_t}{\sigma} = D_{\sigma t} = \frac{1}{E_0} + \left(\frac{1}{E_\infty} - \frac{1}{E_0} \right) \varphi_{\sigma t} \ , \tag{6}$$

where $D_{\sigma t}$ is the flexibility of the polymer material.

Let us illustrate the developed methodology for computational prediction of deformation processes of polymer materials using as an example polyester textile yarn (Fig. 1) prepared from polyester fiber (Fig. 2).

The choice of materials was not by chance. The polyester fiber shown in Fig. 2 is considered a nanoscale development. Its production technology can produce materials with many useful properties. Polyester fiber is opaque and elastic, passes air, and absorbs moisture. It is very soft and does not clump. It is hypoallergenic, biostable, and resistant to soiling. It practically does not accumulate static electricity and has other useful properties.

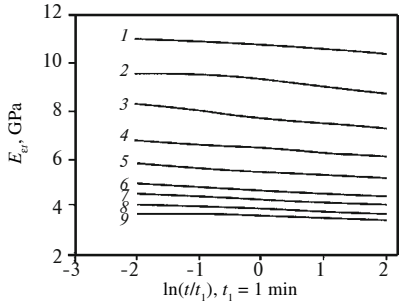

Fig. 3.

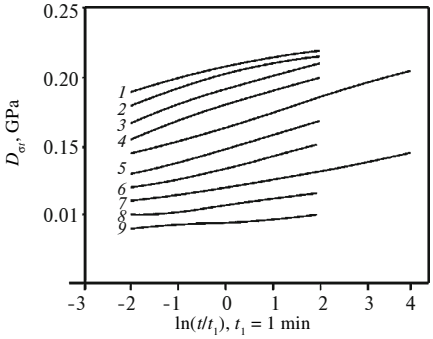

Fig. 4.

Fig. 3. Family of relaxation modulus curves of polyester textile yarn for various deformations (ε, %): 0.5 (1), 1.0 (2), 1.5 (3), 2.0 (4), 2.5 (5), 3.0 (6), 3.5 (7), 4.0 (8), 4.5 (9).

Fig. 4. Family of deformation curves of polyester textile yarn for various stresses (σ, MPa): 194 (1), 182 (2), 170 (3), 158(4), 146 (5), 134 (6), 121 (7), 109 (8), 97 (9), 73 (10).

Polyester fiber is a material that started a qualitative revolution in the textile industry. It is deservedly called "synthetic fiber No. 1" and "21st century material."

Polyester fibers are widely used in textile manufacturing. They are used not only to fabricate clothes but also as raw material for preparing materials for medical and sanitary-hygiene purposes. Microfibers can be used to create unique sports clothing and effective items for skin care.

Chemically, polyester fibers result from the reaction of the diatomic alcohol ethylene glycol with terephthalic acid. The complicated polymerization can produce white or transparent crystals, the main property of which is the viscosity upon heating. The polymer fiber is produced in just this manner from the chemical substance.

The material is prepared at temperatures >260ºC. This guarantees that items made of polyester fibers will be stable. They withstand boiling and most types of modern sterilization of materials [9].

Polyester fibers and materials made of them have many textile and technical characteristics that exceed those of synthetic fibers of another type and production method. They are completely synthetic. This makes them universal with respect to medical applications.

Polyester fibers and items made of them are not of themselves nutritious for microorganisms. The use of such items can considerably reduce the risk of infection during manipulations and surgical operations [10].

The list of applications of polyester fibers is constantly increasing because composites with them can give a finished product a whole bouquet of high-quality consumer attributes, e.g., not only the optimal ratio of cost and quality but also contemporary esthetics, long life, and antibacterial cleanliness. No natural or known chemical material has such a high-quality profile as polyester fiber.

Figure 3 shows an experimentally obtained family of relaxation modulus curves of polyester textile yarn. The relaxation modulus curves in the family had analogous deformation–time behavior, i.e., the curves shifted to shorter times without changing their shape as the stress increased. The deformation family of curves (Fig. 4) also had a force–time analogy property, i.e., the curves shifted to shorter times without changing shape as the stress increased [11].

The equations describing relaxation (Eq. 1) and creep (Eq. 2) can be considered alternatives for each other, although an advantage cannot be given to either of them.

Prediction of the operational processes of uniaxially oriented polymer materials has definite significance for determining their functionality. The more accurate and reliable the prediction is, the more dependable the information obtained about the functional properties of one material or another will be [12].

Prediction of operational processes is the controlling direction for developing recommendations for creating new material structures with given functionality. Digital economics methods can be used to design new material structures with given functionality. Thus, new materials with a particular functionality can be designed much more simply by having a digital library of virtual analogs of exemplary polymer materials and functional properties.

In support of this, special attention is being paid to improving the accuracy of computational prediction of operational processes of polymer materials, the main ones of which are relaxation and creep processes.

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REFERENCES

1. N. V. Pereborova, *Izv. Vyssh. Uchebn. Zaved., Tekhnol. Tekst. Prom-sti.*, No. 2, 93-98 (2022).
2. N. V. Pereborova, *Dizain Mater. Tekhnol.*, No. 1, 154-160 (2022).
3. N. V. Pereborova, E. I. Chalova, and D. A. Ovsyannikov, *Vestn. S.-Peterb. Gos. Univ. Tekhnol. Dizaina (SPbGUTD), Ser. 4, Prom. Tekhnol.*, No. 1, 5-10 (2022).
4. E. I. Chalova and N. V. Pereborova, *Vestn. S.-Peterb. Gos. Univ. Tekhnol. Dizaina (SPbGUTD), Ser. 4, Prom. Tekhnol.*, No. 1, 19-26 (2022).
5. N. V. Pereborova, A. M. Litvinov, and L. V. Titova, *Vestn. S.-Peterb. Gos. Univ. Tekhnol. Dizaina (SPbGUTD), Ser. 4, Prom. Tekhnol.*, No. 2, 5-9 (2022).
6. N. V. Pereborova, *Vestn. S.-Peterb. Gos. Univ. Tekhnol. Dizaina (SPbGUTD), Ser. 4, Prom. Tekhnol.*, No. 2, 16-22 (2022).
7. A. M. Litvinov, A. A. Kozlov, et al., *Izv. Vyssh. Uchebn. Zaved., Tekhnol. Legk. Prom-sti.*, No. 1, 82-87 (2021).
8. N. S. Klimova, A. M. Litvinov, et al., *Izv. Vyssh. Uchebn. Zaved., Tekhnol. Legk. Prom-sti.*, No. 1, 100-105 (2021).
9. N. V. Pereborova, V. I. Vagner, et al., *Izv. Vyssh. Uchebn. Zaved., Tekhnol. Legk. Prom-sti.*, No. 2, 110-114 (2021).
10. N. V. Pereborova, N. S. Klimova, et al., *Vestn. S.-Peterb. Gos. Univ. Tekhnol. Dizaina (SPbGUTD), Ser. 1, Estestv. Tekh. Nauki*, No. 2, 41-51 (2021).
11. N. V. Pereborova, A. A. Kozlov, and S. V. Kiselev, *Vestn. S.-Peterb. Gos. Univ. Tekhnol. Dizaina (SPbGUTD), Ser. 1, Estestv. Tekh. Nauki*, No. 4, 28-33 (2021).
12. N. V. Pereborova, N. S. Klimova, et al., *Izv. Vyssh. Uchebn. Zaved., Tekhnol. Legk. Prom-sti.*, No. 1, 7-13 (2021).