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Relationship between physical, mechanical and thermal properties of flexible chain polymers

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The results of the study on the relationship between the physical, mechanical and thermal properties of linear flexible polymers due to the harmonic and anharmonic components of the interatomic and intermolecular interaction force are presented. Using the example of polyvinyl chloride (PVC), polyvinyl butyral (PVB), polystyrene (PS), it is shown that in the region of $300 \text{ K} \leq T \leq 400 \text{ K}$, the relaxation state of the system is realized due to the mobility of the structural elements, which makes it possible to apply the terms of thermodynamics and statistics of small systems to the properties of the material, and to treat the polymeric state as a special form of condensation of matter. The quantitative relationship between the properties of systems has been established, which is of interest for creating scientific foundations for predicting, obtaining and operating materials under the action of external fields of various nature.

Keywords: polymer, structural element, local equilibrium, oscillator.

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Introduction

In spite of the fact that the mechanical properties of low-molecular weight bodies are determined by the harmonic component of the force of interatomic and intermolecular interaction, and the thermal properties are primarily determined by the anharmonic component, a relationship between some of them has been established [1]. The first attempt to obtain similar dependencies for polymeric bodies was made in [2], where the author pointed out the existence of a relationship between the thermal expansion coefficient and the hardness of a material. However, let alone more complex heterogeneous systems (HS), such a relationship between a number of other physical, mechanical and thermal properties of polymers has not been established and experimentally verified yet. At the same time, scientific research and practical application of polymeric materials have shown that they play an important role in the development of scientific and technological progress with unlimited possibilities. It has been established that the properties of

polymers depend on their composition, structure and test conditions [3]. The energy approach to the study of a set of properties allows to explain the heat capacity, elastic and optical properties of the material from a unified position. It is shown that at high elastic stresses or at high temperatures the displacements of structure elements from the quasi-equilibrium position are large, and consideration of anharmonic components of structure dynamics and kinetics makes it possible to explain thermal expansion, thermal conductivity and other material properties. Accordingly, it appears possible to account for the nonlinear effects of the mobility of structure formation in the forming of a set of material properties, using the theory of energy exchange processes, in particular: matter, momentum, and energy [3]. In general, the transfer phenomenon is one of important branches of science as the research results are important for power, metallurgical, chemical and other industries. At the same time, figuring out the physics of the process, it is important to proceed from the fact that types of physical, chemical and other phenomena, in fact, represent certain varieties of a limited number of laws. Accordingly, the aim of the work is to

establish a quantitative relationship between the physical, mechanical and thermal properties of flexible chain polymers, taking into account the specifics of their behaviour in external force and energy fields.

I. Model. General characteristics, basic concepts

It has been established that the properties exhibited by a polymer, both in the melt and in the solid state, are concentrated in the macromolecule [4]. The peculiarities of the polymer state are most fully manifested in linear and moderately cross-linked polymers [3]. Therefore, we will consider the interrelation of properties in such systems because each structural group in the molecular chain possesses a function which appears in the properties complex of the substance [5]. This function will be based on the statement that there is a series of values and their derivatives which obey the additivity principle. This is due to the fact that the structure of polymers is created by the sequence of functional groups. Macromolecules of linear flexible chain polymers can assume different conformations and form a large system - a macroscopic body with a structure that depends on the mode of physical condensation, their mutual arrangement in space, their internal structure and the nature of interaction (bonding) between them [6]. In this case, a macromolecule has a rather complicated structure characterized by a hierarchy of configuration levels. Since the structure of any physical body is a set of constantly increasing subsystems possessing a certain, usually limited, autonomy, it is expedient, based on statistical physics [7], to introduce the concept of a characteristic particle, a structural element, which forms a certain level of structural organisation. Structural elements of macromolecules are links of chains, and macromolecules of linear polymers are distinguished into a special subsystem, since the terms of thermodynamics and statistics of small systems can be applied to describe their properties [8].

The degree of autonomy of structural elements of a macromolecule depends exclusively on their mobility which is the main physical criterion. In linear flexible chain polymers only fluctuating structural elements with finite lifetime, i.e. microblocks, may exist [9]. As a model we represent them by point masses M_1 , M_2 as atomic groups (for example, in the case of PVC $[-CH_2CHCl-]_n$ the mass of atomic group CH_2 is $M_1 = 23.28 \cdot 10^{-27}$ kg, and group $CHCl$ is $M_2 = 80.46 \cdot 10^{-27}$ kg).

According to [8], these atomic groups are united by bonds, which are characterized by force constants f_1 and f_2 . Considering forces of interaction of two adjacent atomic groups, the equations of motion for two structural elements as $f_1=f_2=f$ can be obtained [8]. When considering a macromolecule in the form of a linear chain each structural element (atomic group) is characterized by two anharmonic force interaction constants of appropriate order. In the case of interatomic interaction these will be force constants of the third, fourth, etc. orders, denoted respectively as g , h , etc. It was shown in [4] that vibrations of a macromolecule are caused by the motion of its atomic groups, and the dynamics of the structural organization of the polymer can be represented in the form of a Lagrange

or Hamilton function. This makes it possible, according to [9], to decompose the potential energy value φ by the degree u of displacement of the structural element near the equilibrium position a in a series up to and including terms of the fourth order:

$$\varphi = \varphi(a) + \frac{1}{2}fu^2 + \frac{1}{3!}qu^3 + \frac{1}{4}hu^4. \quad (1)$$

The equilibrium position a of a structural element is determined by the condition $\varphi' = 0$. The deviation of the distance from a in two neighbouring atomic groups, e.g. n and $(n+1)$, is calculated as

$$r_{n+1} - r_n - a = u_n, \quad (2)$$

In the case of a new energy impact on the system, another state (2) arises, corresponding to the value $a_d = (1+\varepsilon)a$, which is described, according to (1), by a function of the form:

$$\varphi = \varphi(a_d) + au + \frac{1}{2}fu^2 + \frac{1}{3!}qu^3 + \frac{1}{4}hu^4, \quad (3)$$

where the expansion coefficients are equal to:

$$\begin{aligned} e(\varepsilon) &= \varphi'(a_d) = fa\varepsilon + \frac{1}{2}q(a\varepsilon)^2 + \frac{1}{3!}h(a\varepsilon)^3 \\ f(\varepsilon) &= \varphi''(a_d) = f + qa\varepsilon + \frac{1}{2}h(a\varepsilon)^2 \\ q(\varepsilon) &= \varphi'''(a_d) = q + ha\varepsilon \\ h(\varepsilon) &= \varphi''''(a_d) = h. \end{aligned} \quad (4)$$

Consequently, taking into account the influence of anharmonic vibrations of structural elements in the form of force constants f , q , h on the value of heat capacity and thermal conductivity of systems comes down to determining the potential of their interaction.

The potential interaction energy of two isolated molecules can be described by various equations [1]. However, the best agreement with experience is given by the Lennard-Jones potential [4], which defines the potential energy of one macromolecule as a half-sum of pairwise interactions between a given molecule and all other molecules in the phase:

$$\varphi = 4A \left[\left(\frac{a_1}{r} \right)^{12} - \left(\frac{a_1}{r} \right)^6 \right]. \quad (5)$$

According to relation (5), we determine the maximum value of the interaction force between structural elements $= -\partial\varphi/\partial r$, and the condition of its extremum will allow us to calculate the corresponding distance between them. Since

$$\frac{\partial F}{\partial r} = -\frac{\partial^2 \varphi}{\partial r^2} = 24A \left[-26 \frac{a_1^{12}}{r^{14}} + 7 \frac{a_1^6}{r^8} \right], \quad (6)$$

at $r = r_{max}$ (6) we have

$$26 \frac{a_1^{12}}{r_{max}^{14}} = 7 \frac{a_1^6}{r_{max}^8},$$

which corresponds to $r_{max} = a_1(26/7)^{1/6} \approx 1,24a_1$. The equilibrium distance r_p , which corresponds to the

harmonic oscillations of the structural elements of the system, is determined from condition [9]:

$$\frac{12A_n}{r_p^{12}} = \frac{6A_m}{r_p^6}, \quad (7)$$

where $(A_n = Aa_1^{12}, A_m = Aa_1^6)$ is the value of $1,12a_1$.

The value r_p corresponds to the potential energy of the system:

$$\varphi(r_p) = -\eta = -\frac{A_m}{2r_p^6}. \quad (8)$$

Thus:

$$\varphi = \frac{A_m}{12r_p^6} \left[12 \left(\frac{r_p}{r} \right)^6 - 6 \left(\frac{r_p}{r} \right)^{12} \right]. \quad (9)$$

Decomposing φ into a power series (1) of the equilibrium distance between the structural elements and using relations (4), (9), we have:

$$\begin{aligned} f &= \varphi''(r_p) = \frac{36Aa_1^6}{r_p^8} > 0 \\ q &= \varphi'''(r_p) = -756 \frac{Aa_1^6}{r_p^9} < 0 \\ h &= \varphi''''(r_p) = 13356 \frac{Aa_1^6}{r_p^{10}}. \end{aligned} \quad (10)$$

Considering the atoms in the main valence chain as a system of oscillators and considering that the number of atoms having a displacement u is determined by the Boltzmann multiplier $\exp(-\varphi(u)/kT)$, we obtain

$$u = \frac{\int_{-\infty}^{+\infty} u e^{-\varphi(u)kT} du}{\int_{-\infty}^{+\infty} e^{-\varphi(u)kT} du} = \frac{\int_{-\infty}^{+\infty} u e^{\frac{fu^2}{2kT} - \frac{qu^3}{3kT}} du}{\int_{-\infty}^{+\infty} e^{\frac{fu^2}{2kT} - \frac{qu^3}{3kT}} du}, \quad (11)$$

where $e^{\frac{qu^3}{3kT}} = 1 + qu^3/3kT + \dots$

Since the anharmonic correction energy is small compared to the thermal energy : $1/3qu^3 \ll kT$, then

$$u = \frac{q \int_{-\infty}^{+\infty} u^4 e^{\frac{fu^2}{2kT}} du}{3kT \int_{-\infty}^{+\infty} e^{\frac{fu^2}{2kT}} du}, \quad (12)$$

intergrating, we get:

$$u = \frac{qkT}{f^2}. \quad (13)$$

The relative main valence chain distortion of a linear polymer macromolecule per interatomic distance is

$$\frac{u}{a} = \frac{qkT}{af^2} = \alpha T = -\frac{21ka_1^7}{36Aa_1^7}. \quad (14)$$

Consequently, the value of the linear thermal expansion coefficient α is defined as:

$$\alpha = \frac{qk}{af^2} = -\frac{21a_1^7 k}{a_1^7 A}, \quad (15)$$

and it depends on the activation energy (A) of the process as well as the structural characteristics of a_1 substance.

If we consider the elastic deformation of the polymer, then the value of the deformation force is determined accordingly:

$$F = Ea_1 u = fu \quad (16)$$

at the elastic modulus of the polymer

$$E = \frac{f}{a_1} = \frac{36Aa_1^5}{a_1^3}. \quad (17)$$

Considering a macromolecule of a linear polymer as a linear crystal [4], we establish a quantitative relationship between the ultimate strength, ultimate strain of the polymer material and its thermal characteristics. Since the ultimate strength is reached at a strain whose value is $u_{max} = a_{max} - a_1$ determined from the condition $dF/du = 0$, the ultimate relative strain equals $u_{max} = f/2q \approx 1.24a_1$ that is, $a_{max} \approx 2.24a_1$. In this case, the ultimate value of the breaking force is:

$$F_{max} = fu_{max} - qu_{max}^2 = \frac{f^2}{4q}, \quad (18)$$

and the total breaking stress is equal to

$$\sigma_d = \frac{F_{max}}{a_1^2} = \frac{f^2}{4q\pi a_1^2} = \frac{3a_1^2}{7\pi a_1^7} A. \quad (19)$$

The analysis of the obtained dependences shows that the limit characteristics of physical and mechanical properties are additionally determined by the parameter q which characterizes the degree of deviation of the interaction force between atoms or groups of atoms of the main valence chain from the quasi-elastic one, in contrast to the elastic properties. Consequently, q determines not only the physical and mechanical but also the thermal properties of the material.

Taking into account specificity of structural elements, to calculate heat transfer coefficient (λ) of a substance, in our study we use the method of additive interaction of contributions depending on the nature of atomic surroundings in the corresponding molecular groups. According to this method, the value λ of the system can be calculated as [5]

$$\lambda = \sum_{j=1}^n \sum_{g=1}^n \omega_{ij} \lambda_{ij} \quad (20)$$

where ω_{ij} is the overlap coefficient, which accounts for the contact values between groups i and j ; λ_{ij} is the contribution to the value due to the overlap of groups i and j ; n is the number of groups in the system. It should be noted that there is no complete theory that can be used to determine the exact value λ of solutions and solid polymers [10]. Most theoretical and/or semi-empirical relationships are based on Debye's scheme [7] for calculating the value of the heat transfer coefficient, in which the additive quantities are the Rao function, molar heat capacity and volume. However, it should be mentioned that the numerical values of specific polymer characteristics are influenced by external factors [4]. At the same time, molecular processes are of relaxation nature and occur in systems that are in a non-equilibrium

state [11]. Accordingly, when studying the heat transfer process, we use elements of the phenomenological theory of thermodynamics of irreversible processes in the framework of statistical mechanics [7], when the assumed state of the system differs little from the quasi-equilibrium state. The minimal linear dimensions of the subsystems are of the order of the run length of substance carriers. Let us assume that the flexible-chain polymer as a

macroscopic body consists of N structural elements, the motion of which is described by the laws of classical mechanics. Then the Hamilton function ($H(X)$) of the system will be represented as the sum of three components: kinetic energy of elements of mass m , their potential energy in an external field and potential energy of interaction between them [7], that is

$$H(X) = \sum_{1 < i < N} \left[\frac{\overline{P_i^2}}{2m} + U_0(\overline{r}_i) \right] + \frac{1}{2} \sum_{1 < i < N} \Phi(|\overline{r}_i| - |\overline{r}_j|) \equiv \sum_{1 < i < N} \frac{\overline{P_i^2}}{2m} + U(\overline{r}_1, \overline{r}_2, \dots, \overline{r}_N) \quad (21)$$

where $X = (x_1, x_2, \dots, x_N) \equiv (\overline{r}_1, \overline{r}_2, \dots, \overline{r}_N)$ means the totality of the coordinate and momentum values of all the elements of the medium; P_i is the momentum of the particles in the system; $\Phi(|\overline{r}_i| - |\overline{r}_j|) \equiv \Phi(|\overline{r}|) \equiv \Phi_{ij}$ - the interaction of particles is determined by the double sum of the potential energies of the corresponding pairs. Assuming $N \rightarrow \infty$, according to (21), we define the kinetic energy of the system as

$$H(X) - U(\overline{r}_1, \overline{r}_2, \dots, \overline{r}_N) = \frac{3}{2} NkT, \quad (22)$$

where $\frac{3}{2} kT = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{1 < i < N} \frac{\overline{P_i^2}}{2m}$ is the average kinetic energy per structural element; $H(X)$ is the Hamilton function determined by the interaction energy, and is small compared to the Hamilton function of the system and surrounding bodies [7].

It has been found that in the case of insignificant quantum effects, this equation is valid for gases, liquids and solids [13]. From the condition that the size of the selected polymer system (L) is much larger than the run length (l) of the energy (heat) carrier, the small values of r_0, r_m, l (where $l \sim nr_0^2, r_m \sim (l/n)^{1/3}, n = N/V$ is the average density of the body structure elements) follow. This allows, using the approximate Boltzmann equation [3], to express the relation for heat transfer coefficient through parameters ρ, ν, T as [8]

$$j = \frac{dQ}{dFdt} = \lambda \frac{dT}{dl}, \quad (23)$$

where dQ is the amount of heat that passes through an element of isothermal surface dF during time dt ; dT/dl is the temperature gradient. Fulfillment of condition $r_0 \ll r_m \ll l$ gives an opportunity to get a relation for defining the value of internal pressure P of the system as [7]

$$P = \frac{\rho}{m} kT. \quad (24)$$

It should be noted that equation (23) is one of the equations of hydrodynamics [11], as a result of the thermodynamics of non-equilibrium processes [7], and serves as the basis for defining λ as

$$\lambda = \frac{dQ}{dFdt} \frac{dl}{dT}. \quad (25)$$

Using the system of equations (22), (22), (24), after appropriate mathematical transformations, we find that

$$\lambda = \frac{5}{2} \frac{k}{a_l^2} \left(\frac{3kT}{m} \right)^{1/2}, \quad (26)$$

where k is Boltzmann constant; a_l^2 is the effective dimensions of the Kirkwood-Reisman cross section as a source of energy dissipation [12]; m is the mass of the polymer monomer link. Using equations (17) and (26) it follows that

$$\lambda = BE^{2/3}, \quad (27)$$

where $B = \frac{5ka_l^8}{2(36A)^{2/3}} \left(\frac{kT}{m} \right)^{1/2}$. Given the higher order power constants (4), according to [14], we determine the effect of anharmonicity on the molar heat capacity of the system:

$$C_p = 3N_0k \left[1 + kT \left(-\frac{h}{4f^2} + \frac{5g^5}{12f^3} \right) \right]. \quad (28)$$

After substituting the values of f, g, h we have:

$$C_p = 3N_0k \left(1 + kT \frac{2.5a_l^6}{Aa_1} \right), \quad (29)$$

which, using relations (15, 17, 19), makes it possible to additionally obtain analytical relations reflecting the relationship between the physical, mechanical and thermal properties of polymers.

II. Object of the study. Results and discussion

Polyvinyl chloride (PVC) PVC-C70 (Z-10-U), PVC KSR-676 (KARVINIL SR-67), polystyrene (PS) PS-T (GOST 9440-60, UPP-1, UPP-1 concentration in styrene 40 %, pressure 0.1 MN/m², polyvinyl butyral PVB (PS-DS-9439) have been used as the object. The properties of the selected polymers are well studied, which facilitates the interpretation of energy exchange processes in them and allows them to serve as a basis for developing model representations in the study of other systems.

Thermal capacity was investigated on a modified IT-C-400 (GOST 8.001-71), thermal conductivity - IT-400 (GOST 8.001-80), viscoelastic properties - at 0.4 MHz using the pulse method together with the rotating plate method [12]. The temperature range of research is (300 ÷ 400) K. The strength properties of polymers in a glassy

state have been determined using a universal testing machine SZF-1 at a strain rate of 25 mm/min and temperature (300 ÷ 315) K. Deformation of the specimens in compression is accompanied by their brittle fracture. As follows from Fig. 1, a strong increase of α and a decrease of α_d are observed in the transition region between the glassy and highly elastic states for all systems. This dependence is satisfactorily described by the relation which follows from equations (15) and (19)

$$\alpha = C\sigma_d, \quad (30)$$

where $C = (1/V)(k/a^3)$.

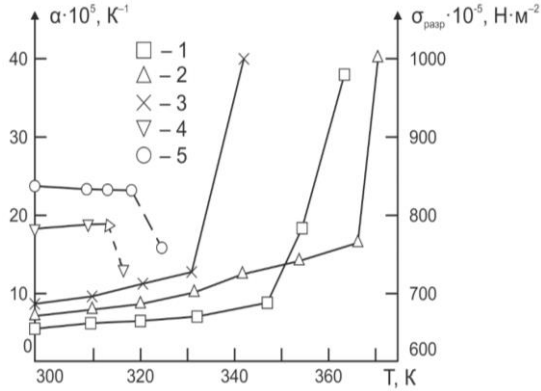


Fig. 1. Temperature dependence of α PVC (1); PS (2); PVB (3) and ultimate compressive strength (σ_d) of PVB (4); PVC (5).

Fig. 2 shows the results of the temperature dependence λ and E of the systems, based on experimental data and calculations carried out according to relations (17) and (26). In the range of 300 K $\leq T \leq$ 400 K there is a typical dependence of $\lambda=f(T)$, $E=\varphi(T)$, which is characteristic of amorphous polymers [14]. At the same time in the whole temperature range a satisfactory agreement between the experimental and calculated values of $\lambda(E)=\Psi(T)$ is observed, confirming the possibility of using the relation (27) to predict the polymer behavior in temperature and mechanical fields. The established relation between the physical, mechanical and thermal properties of flexible-chain polymers is confirmed by the presence of a minimum of thermal stability of the material in the transition region between the glassy and highly elastic state [15]. It should be noted that relatively few polymers have been studied from this perspective. Therefore, it was of interest to investigate the thermal and mechanical stability coefficients of PVC, PVB, PS in the form of entropic capacity (C_p/T), adiabatic $\chi_a=1/\rho v_l^2$ and isothermal ($\chi_T=\chi_a+T\beta^2/\rho C_p$) compressibility. The knowledge of these values made it possible to determine the inverse of the thermal stability determinant of the system:

$$D_c = D^{-1} = \begin{vmatrix} \rho C_p/T & \beta \\ \beta & \chi_T \end{vmatrix}. \quad (31)$$

The calculation D^{-1} was based on experimental data of density, entropicity, volumetric expansion coefficient and isothermal compressibility [12].

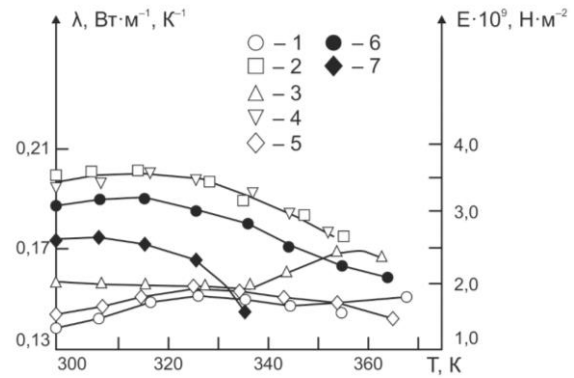


Fig. 2. Temperature dependence of λ and E systems: 1.5 - PVC-S70; 2.4 - PVB; 3 - PS-T; 6 - E - PVC-S70; 7 - E - PVB.

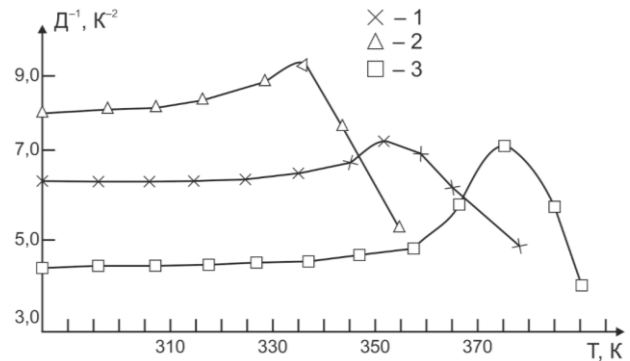


Fig. 3. Temperature dependence of D^{-1} systems: 1 - PVC - KSR-676; 2 - PVB (PH-DS-9439); 3 - PS-T.

Fig. 3 shows that in the region of reduced stability the value of D^{-1} reaches an extreme value. All the curves obtained have a similar shape, but the magnitude of the maximum, its width and position on the temperature scale depend on the type of polymer (a, a_τ, A). This indicates a different nature of the supramolecular ordering and the rate of its degradation. Consequently, the properties of macromolecules (the structural information encoded therein) are transmitted through all subsequent levels of the supramolecular organization of polymers. It is characteristic that in the mesophase area no disappearance or appearance of new physical, mechanical or thermal properties takes place but the change in the character of their temperature dependence. This is due to the destruction of various types of bonds and the appearance of new changes in the system. For example, the PVB under study has $MM = 5 \cdot 10^4$ and contains 20% hydroxyl, 35% acetate and 45% butyral groups. The relative distribution of dipoles in the macromolecule is as follows: C-H (79.60%), O-H (10.40%), C-O (10.0%); this allows the interaction strength of the different dipoles in a particular structure to be calculated [13]. The broadening of the interfacial region (Fig. 3) indicates a slower bond breaking by the temperature field and a shift of the fluctuation region of disordered nuclei of the high-temperature phase to the higher temperatures (340 – 370) K.

Conclusions

Thus, on the basis of research of complex properties of flexible-chain polymers (PVC, PVB, PS) by singling

out the system structure, hierarchy of its subsystems the analytical relationship between physical, mechanical and thermal properties of the material is established. The results obtained can be used as a technology algorithm for prediction, fabrication and using materials in thermal and mechanical fields.

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Взаємозв'язок фізико-механічних і теплофізичних властивостей гнучколанцюгових полімерів

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Наведено результати дослідження взаємозв'язку фізико-механічних і теплофізичних властивостей лінійних гнучколанцюгових полімерів, що зумовлений гармонійною та ангармонійною складовою сили міжатомної та міжмолекулярної взаємодії. На прикладі полівінілхлориду (ПВХ), полівінілбутирало (ПВБ), полістиролу (ПС) показано, що в ділянці $300\text{ K} \leq T \leq 400\text{ K}$, за рахунок рухливості елементів структури реалізується релаксаційний стан системи. Це дає змогу застосувати до властивостей матеріалу терміни термодинаміки і статистики малих систем, а полімерний стан трактувати як особливу форму конденсації речовини. Встановлений кількісний взаємозв'язок між властивостями систем представляє важливий інтерес для створення наукових засад прогнозування, отримання та експлуатації матеріалів в умовах дії зовнішніх полів різної фізичної природи.

Ключові слова: полімер, структурний елемент, локальна рівновага, осцилятор.