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LOCAL VIBRATIONS AND STRUCTURAL DEFECTS IN CARTILAGINOUS TISSUE

Models of the “chain in a thermostat” type, i.e., models on which the statistical physics of macromolecules is based, have been analyzed. It has been noted that these models ignore vibrational thermal motion. A model of the same type, referred to as the elastic-segmental and where the existence of this motion is taken into account, has been proposed. This motion is reduced to bending vibrations localized within a segment. Formulas for the free vibrational energy and deformation caused by local vibrations have been obtained. The proposed model is used to study the influence of local vibrations on the behavior of defects that can arise in cartilaginous tissue. A possible mechanism by which defects disappear under the influence of local vibrations has been considered.

Keywords: cartilaginous tissue, defects, macromolecule, free vibrational energy.

1. Introduction

By definition (see, e.g., Ref. [1–3]), the macromolecule is a molecule consisting of a large number (on the order of 10^3 or more) of atomic groups (links) that are connected to each other by covalent chemical bonds and form a polymer chain. A graph of a macromolecule is presented in Fig. 1, *a*, where links are the graph nodes, and chemical bonds between the links are the graph edges.

The terms “macromolecule” and “chain” are used as synonyms. For a macromolecule, the following inequality holds:

$$\frac{L_m}{b_m} \gg 1, \tag{1}$$

where L_m is the contour length of the chain, and b_m is the link size. According to inequality (1), it is customary (see, e.g., Refs. [1–3]) to consider a macromolecule as a thermodynamic system. As is known (see, e.g., Ref. [4]), statistical physics is based on a general model, on which can be conditionally called “a thermodynamic system in a thermostat”. A partial version of the general model is “a chain in a thermostat” model, which the statistical physics of macromolecules is based (see, e.g., Refs. [1–3]).

Let us consider the features of this model. It is known that in the adiabatic approximation (see, e.g., work [5]), a thermodynamic system can be considered as a set of force centers, particles. For condensed systems, there are two types of thermal motion: vibrational and thermally activated. By definition, the thermally activated motion is a sequence of thermofluctuation events; in each of them, the system passes from one local equilibrium state to another by overcoming an energy barrier. In the course of this transition, a group of particles (a kinetic unit) performs the so-called elementary displacement by means of a jump.

The duration τ_S of an elementary thermofluctuation event is determined (see, e.g., Ref. [6]) by the formula

$$\tau_S = \tau_H \ \exp\left(\frac{\Delta F}{k_{\rm B}T}\right), \tag{2}$$

where $\Delta F = F_H - F_S$, τ_S and τ_H are the average values of the system's residence times in the states characterized by the free energies F_H and F_S, respec-

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tively, T is the temperature, and k_{B} is the Boltzmann constant. A local equilibrium state characterized by the free energy F_S is established in a finite-size region. In terms of the order of magnitude, the time τ_S is equal to the settling time of this state [6]. The value of F_S is determined by the formula

$$F_S = U_S + F_{VS}, \tag{3}$$

where U_S is the potential energy of this region at $T = 0$, and F_{VS} is the free energy of vibrations localized in this region. The temperature T is established in the region mentioned above as a result of interaction of the indicated local vibrations with delocalized vibrations, which play the role of a thermostat [7, 8].

To what extent does the "chain in a thermostat" model agree with the general scenario of thermal motion outlined above?

Models of the "chain in a thermostat"-type, which are used in the statistical physics of macromolecules, can be conditionally divided into two groups. The structural unit in the first group is a segment; therefore the model is called a "segmental model". The segment is a section of a chain along which the correlations in the link arrangement are preserved. The segmental model consists of a sequence of segments connected to each other by hinges (Fig. 1, *b*). The segment length ℓ coincides, in order of magnitude, with the link arrangement correlation radius. Every segment is considered to be absolutely rigid. This implies that the quantity ℓ serves as the spatial scale in the segmental model. This property of the segment can be explained as follows.

A segment plays the role of a kinetic unit. This means that, before the segment starts to move, a local equilibrium state has to be established, and the corresponding settling time is equal to τ_S. This is a time interval during which correlation between the links that compose a segment is established. Thus the time τ_S plays the role of the time scale in the segmental model. Since the segment is in a local equilibrium state at time moments separated by the interval τ_S, when using the τ_S time scale, the segment moves as a whole, i.e., it behaves as an absolutely rigid unit. Therefore, the segmental model is a sequence of rigid segments connected by hinges. It is obvious that vibrations are impossible in such an idealized model.

The structural unit in the models belonging to the second group is a force center. The model consists of a set of such centers connected by a massless thread (Fig. 1, *c*), whence its name "bead model" follows. It is obvious that the zero mass of the thread excludes the appearance of vibrations in this model.

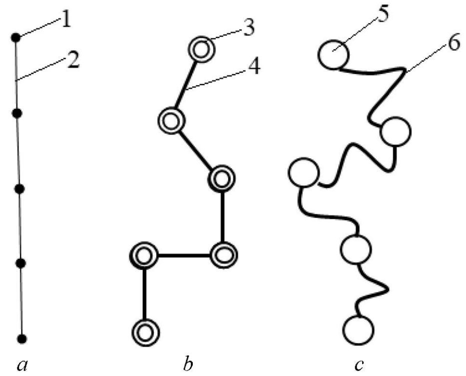

Fig. 1. Macromolecule graph (*a*) and models: segmental (*b*), "bead" model (*c*). Link (*1*), chemical bond (*2*), hinge (*3*), segment (*4*), force center ("bead") (*5*), massless thread (*6*)

The aim of this paper is to propose a variant of the "a chain in a thermostat" model, that allows for the presence of thermally induced vibrations in the chain.

2. Elastic-Segmental Chain Model. Localization Mechanism of Thermal Vibrations

The proposed model belongs to the group of models referred to as segmental. The fundamental difference between proposed model and the others is that in this case, a segment is considered to be an elastic rod. This leads to the model being called elastic-segmental. The chain is now a sequence of elastic rods and, in effect, becomes a waveguide. Generally speaking, the spatial orientation of the segments can be arbitrary. As a result, waves propagating along the chain undergo scattering when passing from one segment to another. The waves satisfying the condition

$$\Lambda \leq 2\ell, \tag{4}$$

where Λ is the wavelength, undergo such intense scattering that they are almost completely reflected from the segment ends, thus becoming localized within the segment itself.

Let us consider a Cartesian coordinate system with axes 1, 2, and 3, where axis 1 is directed along the rod axis. Let $\mathbf{W}$ denote the displacement of rod particles. As is known (see, e.g., Ref. [9]), three types of waves can propagate in the rod: a longitudinal wave, for which the vibrational displacement is the component W_1, and two bending waves, for which the vibrational displacements are the components W_2 and W_3.

3. Thermal Chain Deformation Caused by Local Vibrations

Excitation of thermal vibrations leads to the deformation of segments, which is usually referred to as thermal.

Let us denote by ℓ_0 the segment length at temperature T_0. If the temperature increases to a certain value T, the segment state, to which its length ℓ_0 corresponds, becomes nonequilibrium, and the segment tends to pass into an equilibrium state, in which the segment length is equal to ℓ_T. The value of the segment deformation is determined by the parameter

$$\xi = \ell_0 - \ell_T. \tag{5}$$

It is known (see, e.g., Ref. [10]) that three types of vibrations are realized in a polymer chain: stretching vibrations, associated with changes in the lengths of valence bonds; deformation vibrations, associated with changes in valence angles; and torsional vibrations, induced by rotations of bonds with respect to each other. The indicated vibrations are characterized by the inequalities

$$K_\varphi \ll K_\alpha \ll K_\ell, \tag{6}$$

where K_ℓ, K_α, and K_φ are the force constants of stretching, deformation, and torsional vibrations, respectively.

The force constants K_ℓ and K_α are mainly involved in the propagation of the longitudinal wave, whereas the behavior of bending waves is mainly governed by the force constant K_φ. Let Q denote the bending stiffness of the rod, and h its thickness. Obviously, the bending stiffness of the rod Q, in addition to K_φ, must also depend on the rod thickness h; i.e., it must be a function of these parameters,

$$Q = Q\,(K_\varphi, h). \tag{7}$$

The form of this function can be found using dimensional analysis. According to Ref. [9], Q has the dimension $\mathrm{N\cdot m^2}$, and K_φ has the dimension $\mathrm{N/m}$. Hence, to an accuracy of a constant factor of order one, the following relation holds

$$Q \approx K_\varphi h^3. \tag{8}$$

In the adopted model, a segment is a one-dimensional object, that consists of a set of particles arranged in a line. Thus the thickness of a rod that serves as a segment model is nothing but the size of the particles. According to inequalities (6), the longitudinal stiffness of a segment substantially exceeds its transverse stiffness. This circumstance allows us to assume that the deformation ξ is induced exclusively by bending vibrations. When bending vibrations are excited in a segment, the segment length decreases. This reduction can be regarded as a consequence of the action of a compressive force

$$\xi P = q, \tag{9}$$

on the segment, where q is the segment elasticity coefficient.

As already mentioned, in the adopted chain model, the segments are connected to each other by hinges. According to elasticity theory (see, e.g., Ref. [9]), in this case, the frequencies ω_n of bending vibrations are described by the formula

$$\omega_n = \omega_{0n}\sqrt{1 - Pa_n} \quad (n = 1, 2, .., M-1), \tag{10}$$

where M is the number of particles in the segment,

$$\omega_{0n} = n^2\pi^2\sqrt{\frac{Q}{ml_0^4}}, \tag{11}$$

$$a_n = \frac{l_0^2}{n^2\pi^2 Q}, \tag{12}$$

and m is the chain mass per unit length. In the proposed model, the local equilibrium state discussed in the Introduction, is a state of a subsystem of vibrations localized within a segment. A definite value of free energy can be ascribed to this subsystem only if the inequality $M \gg 1$ is satisfied. Therefore, the proposed model can be applied only to rigid-chain polymers.

Using the general formula that defines the free energy in solid-state physics (see, e.g., Ref. [5]), we can write the free vibrational energy of the segment F_{VS} in the form

$$F_{VS} = 2k_\mathrm{B}T\sum_{n=1}^{M-1}\ln\left(2\sinh\frac{\hbar\omega_n}{2k_\mathrm{B}T}\right), \tag{13}$$

where $\hbar = h/(2\pi)$, and h is Planck's constant. The factor 2 appears on the right-hand side of this formula due to the existence of two bending waves in the segment. Assuming that the condition

$$\frac{\hbar\omega_n}{2k_\mathrm{B}T} \ll 1 \tag{14}$$

is fulfilled, we rewrite formula (13) in the form

$$F_{VS} = 2k_\mathrm{B}T\sum_{n=1}^{M-1}\ln\frac{\hbar\omega_n}{k_\mathrm{B}T}. \tag{15}$$

Substituting equality (10) into formula (15), we obtain

$$F_{VS} = 2k_\mathrm{B}T\sum_{n=1}^{M-1}\ln\frac{\hbar\omega_{0n}}{k_\mathrm{B}T} + F'_{VS}, \tag{16}$$

where

$$F'_{VS} = k_\mathrm{B}T\sum_{n=1}^{M-1}\ln(1-Pa_n). \tag{17}$$

Provided the inequality

$$Pa_n \ll 1, \tag{18}$$

let us rewrite formula (17) as follows:

$$F'_{VS} = -k_\mathrm{B}TP\sum_{n=1}^{M-1}a_n. \tag{19}$$

Substituting expression (12) into formula (19), we obtain

$$F'_{VS} = -k_\mathrm{B}TP\frac{\ell_0^2}{\pi^2 Q}\sum_{n=1}^{M-1}\frac{1}{n^2}. \tag{20}$$

Since

$$\sum_{n=1}^{M-1}\frac{1}{n^2} \approx \sum_{n=1}^{\infty}\frac{1}{n^2} = \frac{\pi^2}{6}, \tag{21}$$

we can rewrite formula (20) in the form

$$F'_{VS} = -k_\mathrm{B}TP\frac{\ell_0^2}{6Q}. \tag{22}$$

The increment F'_S of the segment free energy associated with the force P is determined by the formula

$$F'_S = U'_S + F'_{VS}, \tag{23}$$

where U'_S is the increment of the segment potential energy caused by the action of the force P. Bearing in mind formulas (9), (22), and the obvious inequality

$$\xi/\ell_0 \ll 1, \tag{24}$$

we rewrite equality (23) in the form

$$F'_S = \frac{1}{2}q\xi^2 - k_\mathrm{B}Tq\xi\frac{\ell_0^2}{6Q}. \tag{25}$$

From the condition of segment equilibrium,

$$\left.\frac{\partial F'_S}{\partial\xi}\right|_T = 0, \tag{26}$$

we find the equilibrium value $\xi = \xi_T$ associated with local vibrations,

$$\xi_T = \frac{k_\mathrm{B}T\ell_0^2}{6Q}. \tag{27}$$

Accordingly, for the relative thermal deformation of the segment,

$$\varepsilon = \frac{\ell - \ell_0}{\ell_0}, \tag{28}$$

and taking equalities (5) and (27) into account, we obtain the formula

$$\varepsilon = -\beta T, \tag{29}$$

where

$$\beta = \frac{k_\mathrm{B}\ell_0}{6Q}. \tag{30}$$

Let us evaluate β. The value $K_\varphi \approx 3.4$ N/m is taken from Ref. [10]. Adopting the values $h = 3\times10^{-10}$ m, $\ell_0/h = 30$, and using formulas (8) and (30), we obtain $\beta = 2.2\times10^{-4}$ 1/degree.

Hence, according to formula (29), if the temperature increases and thermal vibrations are excited, the segment length and, therefore, the contour length of the chain decrease.

4. Mechanism of Defect Formation and Regeneration of Cartilage Tissue. Influence of Local Vibrations

Let us consider an example of the application of the proposed model. There is a class of polymer systems called hydrogels; see, e.g., Ref. [11]. They consist of a polymer and water, with the polymer chains forming a framework. Such systems include (see, e.g., Ref. [12]) the cartilaginous tissue of humans. The polymers that constitute the cartilaginous tissue are collagen (10–12%) and proteoglycans (7–8%). Almost

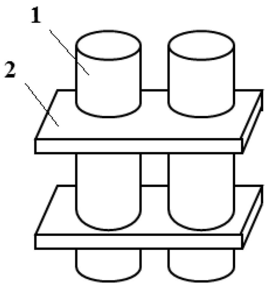

Fig. 2. Schematic diagram of the cartilaginous tissue structure: collagen fibers(*1*), proteoglycan interlayers (plates) (*2*)

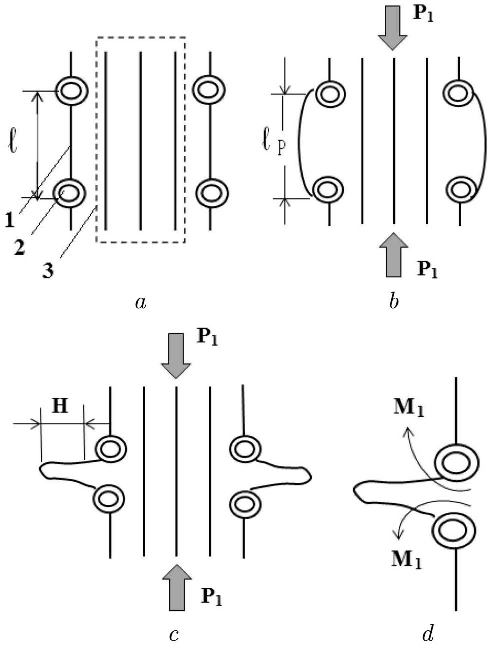

Fig. 3. Shell model of the fiber: undeformed fiber (*a*), segment (*1*), hinge (*2*), elastic filler (*3*); fiber at the moment of stability loss (*b*); formation of a fiber defect (*c*), bending moments arising in the defect as the temperature increases (*d*)

the entire remaining part of the tissue is water [12]. It is known [12] that collagen chains form fibers, with proteoglycan chains located between them. A variant of the cartilaginous tissue structure proposed in Ref. [13], is shown in Fig. 2.

One of the problems discussed in the medical literature is tissue damage (defect) that appears under the action of an external load; see, e.g., Ref. [14]. The specific form of defect remains undefined. Let us consider a possible mechanism for the formation of such defects.

In elasticity theory [15], there exists a model known as “a cylindrical shell with an elastic filler”. We use this model to describe the behavior of the fiber, assuming the thickness of the shell wall to be equal to the chain thickness h. This model is referred to as the “shell model”. It is exhibited in Fig. 3, *a*; the thick lines depict chains, and the dashed lines mark the area occupied by an elastic filler (as such a filler, we will consider chains located inside the shell).

Let a compressive force P_1 act along the fiber axis, and let this force reach a threshold value at which the cylindrical shape of the shell loses its stability. At the moment of stability loss, when the deformations remain small so that they can be calculated using linear elasticity theory, besides the cylindrical shape, a wavy shape becomes possible (it is schematically depicted in Fig. 3, *b*). The corresponding value of P_1 is the bifurcation point [15].

Let us return to the elastic-segmental model. As can be seen from Fig. 3, *b*, the wavy shape of the shell for the chains composing the shell means the formation of “humps”. As already mentioned, this model is a sequence of segments connected by hinges (in Fig. 3, *b*, the latter are shown as double circles). A hinge does not transmit a bending moment, so the length of the chain section on which the “hump” appeared, i.e., the distance between the segment ends, decreases and becomes equal to ℓ_P (Fig. 3, *b*).

Thermal vibrations localized within the segment, facilitate the loss of the cylindrical shape stability; in effect, according to elasticity theory, they reduce the threshold value of P_1. The main contribution to this effect is provided by vibrations with the wavelength $\Lambda = 2\ell$ and the maximum amplitude. Due to this circumstance, the segment acquires the shape depicted in Fig. 3, *b*.

However, the process is not restricted to small deformations. In reality, the loss of stability is accompanied by large deformations, therefore the segment shape shown in Fig. 3, *b* should be regarded as transient. Large deformations are calculated using nonlinear elasticity theory [15].

The final segment shape can be envisaged using qualitative considerations. As already mentioned, the transient shape shown in Fig. 3, *b* was formed because the distance between the segment ends decreases from ℓ to ℓ_P. To obtain the final shape, this distance must be reduced further. This reduction continues until the opposite parts of the segment meet. As a result, a section of length H is formed (Fig. 3, *c*), where the indicated parts become interconnected via interchain bonds. Owing to these bonds, after the action of the force P_1 terminates, the fiber continues to maintain its shape, as is shown in Fig. 3, *c*. Therefore, there appears a defect in the fiber.

One of the methods used to treat damaged cartilaginous tissue is the application of heat-transfer agents (paraffin, ozokerite, mud therapy) to the affected area; see, e.g., Ref. [14]. Under the influence of heat transfer agents, the temperature in the damaged area increases. It is believed that this action leads to peripheral vasodilation, enhanced hemodynamics and lymphatic drainage, and activation of metabolism, which favors the regeneration of cartilaginous tissue.

To our knowledge, the molecular mechanism of tissue regeneration has not been discussed in the literature. Based on the defect model shown in Fig. 3, the following regeneration mechanism can be proposed. An increased temperature in the damaged area leads to an increase in the intensity of local thermal vibrations in this area and, in particular, in the segment where the defect is located. The contour length of the chain section corresponding to the mentioned segment decreases in this case, as required by formula (29). As a result of such a decrease, bending moments M_1 arise in the chain (see Fig. 3, *d*), which tend to break the intermolecular bonds existing in the section of length H. After these bonds are broken, the segment returns to its original normal position (see Fig. 3, *a*).

Hence, local thermal vibrations play a dual role with respect to defects. On the one hand, if a compressive force acts on the fiber, these vibrations contribute to the loss of stability, which leads to the formation of defects. On the other hand, in the absence of an external force and temperature growth, local vibrations contribute to the disappearance of defects, thereby stimulating the regeneration of cartilaginous tissue.

5. Conclusions

The statistical physics of macromolecules is based on the model “a chain in a thermostat”, in which the existence of vibrational thermal motion is ignored. A variant of this model proposed in this work and is referred to as the elastic-segmental model, makes it possible to take this motion into consideration. A distinctive feature of the proposed model is that it treats a segment as an elastic rod. In this model, a segment of a polymer chain is a section of the chain where local equilibrium exists. The free energy of this local equilibrium state is equal to the sum of the potential energy of the particles at temperature T_0 and the free energy of vibrations localized within the segment. Localization occurs due to the scattering of thermal waves at the segment ends. The vibrational free energy is mainly determined by bending waves. As a result, the segment undergoes contraction when thermal vibrations are excited.

Local vibrations play a positive role in the process of cartilage regeneration. The latter includes fibers consisting of collagen chains. Under the action of a compressive force directed along the fiber axis, defects can appear in these chains, as a consequence of the loss of stability of the cylindrical shape of the fiber. Local vibrations play a dual role with respect to such defects. On the one hand, under the action of a compressive force, these vibrations contribute to the aforementioned loss of stability. On the other hand, when the external force ceases, the chain contraction caused by local vibrations contributes to the disappearance of defects and, consequently, the regeneration of damaged cartilaginous tissue.

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ЛОКАЛЬНІ КОЛИВАННЯ ТА СТРУКТУРНІ ДЕФЕКТИ ХРЯЩОВОЇ ТКАНИНИ

Аналізуються моделі типу "ланцюг в термостаті", тобто ті моделі, на яких ґрунтується статистична фізика макромолекул. Відмічається, що ці моделі ігнорують наявність коливального теплового руху. Пропонується модель цього ж типу, названа пружно-сегментальною, в якій існування згаданого руху враховане. Цей рух зводиться до вигинних коливань, локалізованих в межах сегмента. Отримано формулу для вільної коливальної енергії та деформації, спричиненої локальними коливаннями. Запропонована модель використовується при вивченні впливу локальних коливань на поведінку дефектів, які можуть виникати в хрящовій тканині. Розглянуто можливий механізм, завдяки якому під дією локальних коливань відбувається зникнення дефектів.

Ключові слова: хрящова тканина, дефекти, макромолекула, вільна коливальна енергія.