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STRAIN FLUCTUATIONAL THEORY OF ELASTIC CONSTANTS OF NEMATIC ELASTOMERS

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In this communication some aspects of strain fluctuation theory of linear elasticity of nematic elastomers are represented

For description of the elastic properties of elastomers the stress ensemble is used. The distribution function for this ensemble is obtained by means of the method of maximum informational entropy. At first we introduce the microscopic field of displacements [1] as

$$\hat{u}_i(x) = \sum_{\nu=1}^{N} u_i^{\nu} \delta(x - x^{\nu}) \tag{1}$$

and the we construct the microscopic tensor of deformation (for simplicity we consider the linear case)

$$\hat{\varepsilon}_{ik} = \frac{1}{2}\left(\frac{\partial \hat{u}_i}{\partial x_k} + \frac{\partial \hat{u}_k}{\partial x_i}\right) \tag{2}$$

Mean value of this tensor is

$$\langle \hat{\varepsilon}_{ik} \rangle = n\varepsilon_{ik}, \tag{3}$$

where

$$\varepsilon_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right) \tag{4}$$

is macroscopic tensor of deformation, n is the particle number density.

Quasiequilibrium distribution function defined as

$$\rho_q = \exp\left[\Phi - \int dx \beta(x,t)\left(\hat{H}(x) - E_{ik}\hat{\varepsilon}_{ik}\right)\right] \tag{5}$$

$E_{ik} = \tau_{ik}^0 \beta n^{-1}$, τ_{ik}^0 is the stress tensor, $\beta = kT$, k is Boltzmann constant.

The expression type (5) may be apply for the nonlinear measure of deformation [2–5].

In linear approximation we have

$$\rho_q = \rho_0\left[1 - \int d\overline{x}'\left(\hat{H}(\overline{x}') - \langle\hat{H}\rangle_0\right)(\beta - \beta_0) + \int E_{ik}(x')\hat{\varepsilon}_{ik}(x')dx'\right] \tag{6}$$

Using this distribution function we obtain

$$\langle \hat{\varepsilon}_{ij} \rangle = \int E_{kl}(x')\langle \hat{\varepsilon}_{ij}(x)\hat{\varepsilon}_{kl}(x')\rangle dx' \tag{7}$$

or in the local approximation

$$n\varepsilon_{ij} = E_{kl}\int \langle \hat{\varepsilon}_{ij}(x)\hat{\varepsilon}_{kl}(x')\rangle dx', \tag{8}$$

where $\int \langle \hat{\varepsilon}_{ij}(x)\hat{\varepsilon}_{kl}(x') \rangle dx'$ is correlation function of the strains fluctuation.
Therefore

$$\varepsilon_{ij} = B_{ijkl}(x)\tau^0_{kl}(x), \qquad (9)$$

where

$$B_{ijkl} = \beta n^{-2} \int \langle \hat{\varepsilon}_{ij}(x)\hat{\varepsilon}_{kl}(x') \rangle dx' \qquad (10)$$

is the tensor of the isothermal elastic compliances.

The tensor of the elastic module K_{ijkl} connected with the tensor of compliances the next relation

$$B_{ijmn} K_{mnkl} = \delta_{ik}\delta_{jl} \qquad (11)$$

It is very important that the tensor of compliances defined by the correlation function of the strain fluctuations.

Now we consider the simple case of the isotropic medium. Then we have

$$\varepsilon_{12}(x) = \mu^{-1}\tau_{12}, \qquad (12)$$

where μ is shear modulus

$$\mu = \frac{kTn^2\nu}{\iint \langle \hat{\varepsilon}_{12}(x)\hat{\varepsilon}_{12}(x') \rangle dx'dx}. \qquad (13)$$

In liquid case $\varepsilon_{12} \to \infty$, and therefore $\mu \to 0$. That is the shear deformation ε_{12} is the soft mode, ν is the body volume.

It is interesting that in case of the no compressibility of elastomers when Tr $\varepsilon_{ij} = \varepsilon_{ii} \to 0$ we obtain according to (10) that compressibility also go to zero.

In isotropic ase the relations between elastic moduli and corresponding compliances directly follows from formulas [7]

$$\tau_{ij} = K\varepsilon_{ll}\delta_{ij} + 2\mu\left(\varepsilon_{ij} - \frac{1}{3}\delta_{ij}\varepsilon_{ll}\right), \qquad (14)$$

$$\varepsilon_{ij} = \frac{1}{9K}\delta_{ij}\tau_{ll} + \frac{1}{2\mu}\left(\tau_{ij} - \frac{1}{3}\delta_{ij}\tau_{ll}\right). \qquad (15)$$

Then we obtain the expressions for bulk elastic modulus K and for shear modulus (see 13)

$$9K = \frac{n^2kT\nu}{\iint \langle \hat{\varepsilon}_{ll}(x)\hat{\varepsilon}_{kk}(x') \rangle dx'dx}. \qquad (16)$$

The Poisson's ratio defined by [7]
$$\nu = (3K - 2\mu)/2(3K + \mu) \qquad (17)$$

At calculation corresponding correlation functions in (13) and (16) it may occur the next results.

In case, when $3K < 2\mu$, $\nu < 0$ and at $K = 0$ (the compressibility is infinity) $\nu = -1$, at $K \to \infty$ or $\mu \to 0$ $\nu \to \frac{1}{2}$.

It should be noted that in the work [8] the detailed and stimulated review on the materials with negative Poisson ratio is represented.

In our works in addition and in contrast to the works considered in [8] we develop the molecular statistical theory of the elastic properties of materials which may possess the negative Poisson ratio.

For nematic elastomers we have the nest structure tensor of compliances

$$B_{ijkl} = B_1 \delta_{ij}\delta_{kl} + B_2 \delta_{ik}\delta_{jl} + B_3 \delta_{il}\delta_{jk} + B_4 \left(\delta_{ij} n_k n_l + \delta_{kl} n_i n_j \right) +$$

$$+ B_5 \delta_{ik} n_j n_l + B_6 \left(\delta_{il} n_j n_k + \delta_{jk} n_i n_l \right) + B_7 \delta_{jl} n_i n_k + B_8 n_i n_j n_k n_l$$

and the tensor of elastic module have the same structure

$$K_{ijkl} = K_1 \delta_{ij}\delta_{kl} + K_2 \delta_{ik}\delta_{jl} + K_3 \delta_{il}\delta_{jk} + K_4 \left(\delta_{ij} n_k n_l + \delta_{kl} n_i n_j \right) +$$

$$+ K_5 \delta_{ik} n_j n_l + K_6 \left(\delta_{il} n_j n_k + \delta_{jk} n_i n_l \right) + K_7 \delta_{jl} n_i n_k + K_8 n_i n_j n_k n_l .$$

With help of the relation (11) we obtain formulas connected module K_i and coefficient of compliances B_i.

For example

$$K_1 = \frac{B_1 \left(B_5 + 2B_6 + B_7 + B_8 \right) - B_4^2 + B_1 \left(B_2 + B_3 \right)}{T},$$

$$K_2 = \frac{B_2}{B_2^2 - B_3^2} \quad K_3 = -\frac{B_3}{B_2^2 - B_3^2},$$

$$K_4 = \frac{-B_1 \left(B_5 + 2B_6 + B_7 + B_8 \right) + B_4^2 + B_4 \left(B_2 + B_3 \right)}{T},$$

$$K_5 = \frac{2B_2 B_3 B_6 - B_2 B_5 B_7 + B_2 B_6^2 - B_2^2 B_5 - B_3^2 B_7}{A},$$

$$K_6 = \frac{B_2 B_3 B_7 + B_3 B_5 B_7 + B_2 B_3 B_5 - B_3 B_6^2 - B_3^2 B_6 - B_2^2 B_6}{A},$$

$$K_7 = \frac{2B_2 B_3 B_6 - B_2 B_5 B_7 + B_2 B_6^2 - B_2^2 B_7 - B_3^2 B_5}{A},$$

where

$$A = \left(B_3^3 - B_2 B_6^2 - B_2 B_3^2 - B_3 B_5 B_7 + B_2^2 B_7 - B_2 B_3 B_5 - B_2 B_3 B_7 \right.$$

$$+ 2B_3^2 B_6 - 2B_2 B_3 B_6 + B_2^2 B_5 + B_3 B_6^2 - B_2^2 B_3 + B_2^3 + B_2 B_5 B_7 \left. \right)\left(B_2 + B_3 \right),$$

$$T = \left(B_2 + B_3 \right)^2 \left(-3B_1 - 2B_4 - B_5 - 2B_6 - B_7 - B_8 \right)$$

$$+ \left(B_2 + B_3 \right)\left(-2B_1 \left(B_3 + 2B_6 + B_7 + B_8 \right) - 2B_2 B_3 + 2B_4^2 \right)$$

$$- \left(B_2^3 + B_3^3 \right).$$

The modules K_8 is not shown in connection witch bulkiness of expressions.

For nonlinear elastic extension of elastomers the law of this deformation defined by formula [9]

$$P = \mu \left[\left(b_\parallel \lambda - b_\perp \lambda^{-2} \right) - \alpha \left(b_\parallel^{3/2} \lambda^2 - b_\perp^{3/2} \lambda^{-5/2} \right) + \beta \left(b_\parallel^{3/2} \lambda^3 - b_\perp^3 \lambda^{-3} \right) \right], \qquad (18)$$

where $b_\perp = a/l_\perp$, $b_\| = a/l_\|$, a is effective length of monomer, $l_\| = a(1+2Q)$, $l_\perp = a(1-Q)$, Q is the scalar order parameter, λ is multiplicity stretch of material fibre, P is force per unit nondeformation area.

Let us remove in [9] the next misprint: all the numerical values α must be positive, instead of $\alpha = 0,515$ must be $\alpha = 1,515$.

In formula (13) above work instead of $-\alpha\left(2^{-3/2}\lambda^2 2^{-3k}\right)$ must be $-\alpha 2^{-3/2}\lambda^2$.

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