CRITICAL PHENOMENA SOFT MODES AND NEGATIVE POISSON' RATIO

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The article phenomena, soft modes and negative Poisson' ratio are considered on bases at statistical theory

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

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

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

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

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

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

$E_{ik} = \tau_{ik}^0 \beta n^{-1}$, 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

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

Using this distribution function we obtain

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

or in the local approximation

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

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

Therefore

$$\varepsilon_{ij} = B_{ijkl}(x)\tau_{kl}^0(x), \tag{9}$$

where

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

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

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

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

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

where μ is shear modulus

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

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]

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

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

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

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

The Poisson’s ratio defined by [7]

$$\nu = (3K - 2\mu) / 2(3K + \mu). \quad (17)$$

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 shod be noted that in the work [8] the detailed and stimulated review or materiel with negative Poisson’s ratio ism represented.

Let as for analyses of formula (16) take into account the low of conservation

$$n - n_0 = -n \operatorname{div} u, \ \operatorname{div} u = \varepsilon_{ii} \quad (18)$$

Besides we used the relation (3).

The quantity $\Delta n = n - n_0$ a fluctuation of density or concentration.

The expression (16) may be rewrite the next manner

$$9K = \frac{kTn^2}{\int \langle \Delta n(0) \Delta n(r) \rangle dr} \quad (19)$$

and we find that denomination is the correlation of density (concentration) which is diverge at approach to the critical point.

In result bulk elastic modulus goes to zero and according to (17) Poisson's ratio comes to minus one (–1).

Correlation function mae be represented in another form

$$G(r) = \langle n(0)n(r)\rangle - n^2 = n^2\left(g(r) - 1 + \frac{1}{n^2}\delta(r)\right) \tag{20}$$

where g(r) is traditional binary distribution function.

Near critical point g(r)–1 the Orstein-Zernike form

$$g(r) - 1 = \frac{\xi}{4\pi r}\exp\left(-\frac{r}{\xi}\right) \tag{21}$$

Now the quantity 9K is

$$9K = \frac{kT}{\xi^3} \tag{22}$$

where ξ is correlation length, which goes to infinity at approaching to critical point. Thereof in this case $K \to 0$ and $\nu \to -1$.

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

$$P^* = \left(b_\parallel\lambda - b_\perp\lambda^{-2}\right) - \alpha\left(b_\parallel^{3/2}\lambda^2 - b_\perp^{3/2}\lambda^{-5/2}\right) + \beta\left(b_\parallel^{3/2}\lambda^3 - b_\perp^3\lambda^{-3}\right), \tag{23}$$

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

The examples of calculation by formula (23) represented on figures

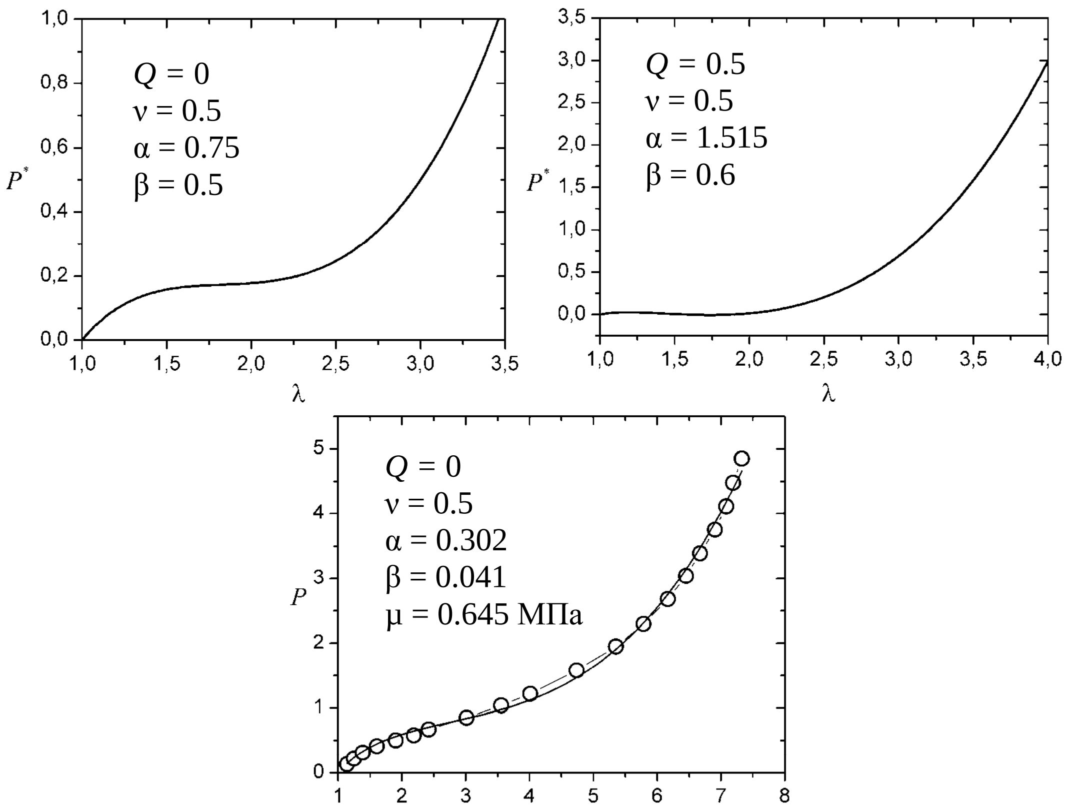

Fig. 1

In an extension of some the polymers, for example DNA molecule and nematic elastomers on the extensions curve the soft modes appears in form plateau. This means that for deformation in limits plateau Young modules and balk modules are zero. Therefore the Poisson’s ratio is negative and may by equal unit.

It is very impotent generalize theory of nematic elastomets on cases when $\nu < 0$ or $\nu \neq 0.5$.

For this end instead of condition volumes invariance we mast use the condition variability a volume. The corresponding relation is

$$\lambda_x \lambda_y \lambda = 1 + (\lambda - 1)(1 - 2\nu), \ \lambda \equiv \lambda_z, \tag{24}$$

At $\nu = 0.5$ we obtain the condition invariants volume $\lambda_x \lambda_y \lambda = 1$.

The equation of stretch of nenatical elastomer for $\nu \neq 0.5$ have the form

$$\begin{aligned} P^* &= b_{\parallel}\lambda - b_{\perp} d^2 \lambda^{-2} + b_{\perp}(1 - 2\nu)\lambda^{-1} - \\ &-\alpha\left[b_{\parallel}^{3/2}\lambda^2 - b_{\perp}^{3/2} d^3 \lambda^{-5/2} + b_{\perp}^{3/2} d (1 - 2\nu)\lambda^{-3/2}\right] + \\ &+\beta\left[b_{\parallel}^2 \lambda^3 - b_{\perp}^2 d^4 \lambda^{-3} + b_{\perp}^2 d^2 (1 - 2\nu)\right], \end{aligned} \tag{25}$$

where $d = \sqrt{1 + (\lambda - 1)(1 - 2\nu)}$.

The parameters α and β find from experiment. Results of calculations at υ positive and negative represent Belov. at Q = 0.1 and Q = 0.3.

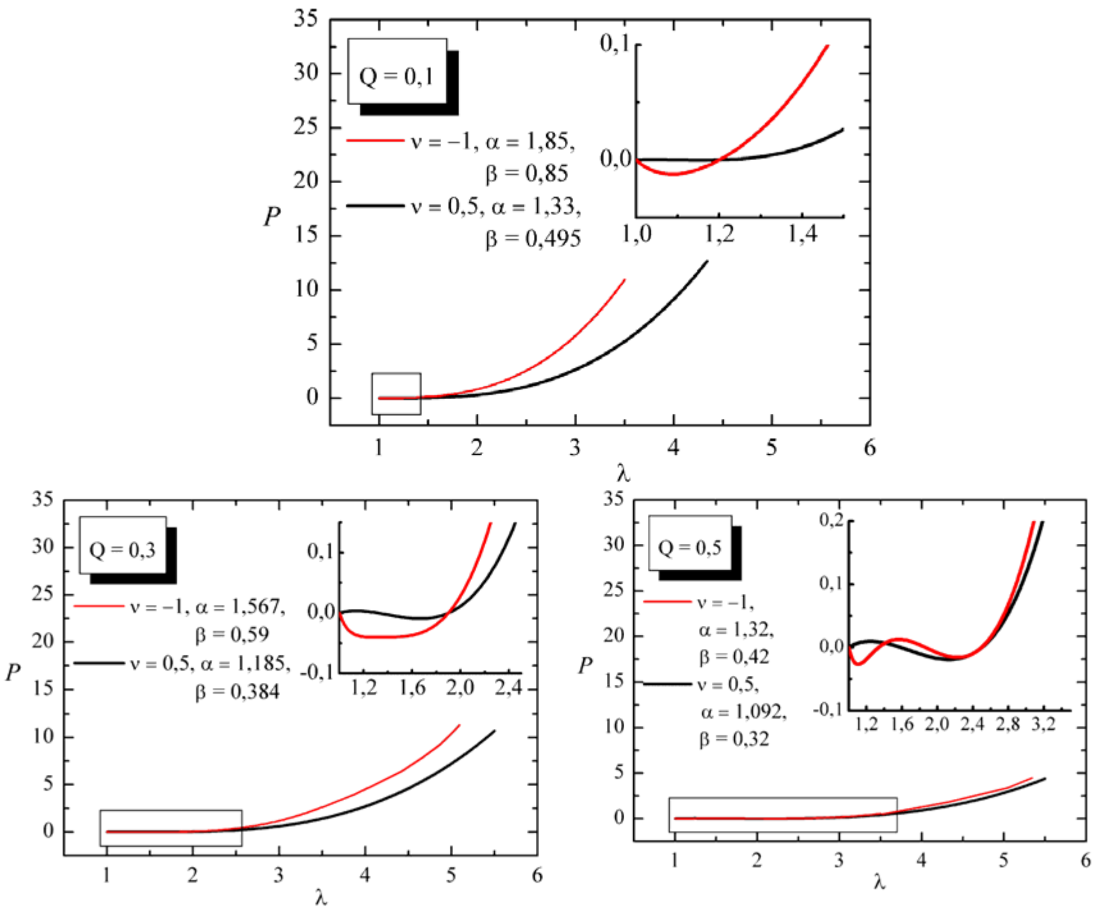

Fig. 2

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