The Lecture Contains

"Mechanics of the Cell" by David Boal, Cambridge University Press, 2002, Cambridge, UK

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Three dimensional networks

We will consider here free energy of deformation of both isotropic materials in three dimension and those with four-fold symmetry. We have shown earlier that in a generalized situation, a three dimensional system under stress is characterized by $3^4 = 81$ number of elastic moduli C_{ijkl}; for two dimension, the number of moduli is $2^4 = 16$. The number of these elastic constants however decreases because of symmetry in the system. For example, since the components of strain u_{ij} are symmetric with respect to the exchange between the subscript pairs (i, j) , (k, l) and (ij, kl), we have the relations $C_{ijkl} = C_{jikl} = C_{ijlk}$ and $C_{ijkl} = C_{klij}$ which diminish the number of independent moduli to 21. The number of moduli gets further reduced for isotropic materials for which the strain components remain invariant for arbitrary rotations. In fact, there are only two quadratic combinations for strain tensor that remain independent with respect to rotation of the axes: $\sum_{i,j} u_{ij}^2$ and tru. Therefore the free energy density function can be written as

$$\Delta\Pi = \mu \sum_{i,j} \left(u_{ij} - \delta_{ij}\, tru/3\right)^2 + 1/2\, K_V (tru)^2 \tag{40.1}$$

Where K_V is the volume compression modulus and μ is the shear modulus of the material. Thus the isotropic system requires two moduli in order to describe its strain energy density function. It can be shown that a system with hexagonal symmetry requires five independent elastic constants. Similarly a cubic system requires three moduli as observed in its expression of free energy,

$$\Delta\Pi = \frac{C_{xxxx}}{2}\left(u_{xx}^2 + u_{yy}^2 + u_{zz}^2\right) + C_{xxyy}\left(u_{xx}u_{yy} + u_{yy}u_{zz} + u_{zz}u_{xx}\right) + 2C_{xyxy}\left(u_{xy}^2 + u_{yz}^2 + u_{zx}^2\right) \tag{40.2}$$

Combining elastic moduli and strain tensor components, above equation is written as,

$$\Delta\Pi = \frac{K_V}{2}\left(u_{xx} + u_{yy} + u_{zz}\right)^2 + \frac{\mu'}{3}\left(\left(u_{xx} - u_{yy}\right)^2 + \left(u_{yy} - u_{zz}\right)^2 + \left(u_{zz} - u_{xx}\right)^2\right) + 2\mu_s\left(u_{xy}^2 + u_{yz}^2 + u_{zx}^2\right) \tag{40.3}$$

where, $K_V = \dfrac{C_{xxxx} + 2C_{xxyy}}{3}$, $\mu' = \dfrac{C_{xxxx} - C_{xxyy}}{2}$, $\mu_s = C_{xyxy}$

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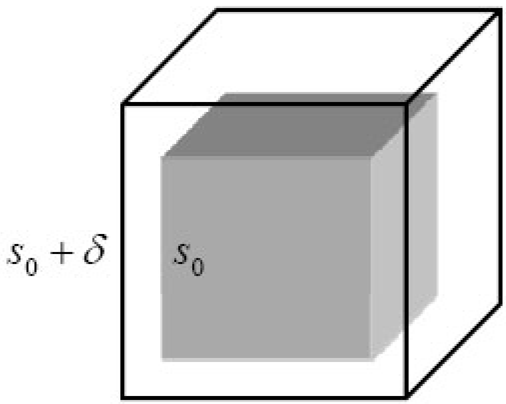
Three dimensional networks (contd...)

We will like to explore how these moduli are related to microscopic structure of a material. We will consider a network of identical springs, each having a potential energy $V(s)\frac{k_{sp}}{2}(s-s_0)^2$, where k_{sp} is the spring constant and s_0 is the unstretched length of the spring. The figure shown below depict that all springs change their length from s_0 to $s_0+\delta$, i.e. the cube undergoes pure compression with the diagonal elements of the strain tensor defined as $u_{xx}=u_{yy}=u_{zz}=\delta/s_0$, the off-diagonal elements are all zero.



Then the change in free energy density is obtained from equation 40.3 as,

$$\Delta\Pi=\frac{9K_V}{2}\left(\frac{\delta}{s_0}\right)^2 \qquad (40.4)$$

How many springs are there per unit cell? The cubical unit cell shown above consists of a single vertex (each of the eight vertices of the cell is shared by eight neighbouring cells) and three springs (each of the twelve chains of the cell is shared by four neighbouring cells). Therefore, because of the deformation of the cell, change in potential energy is deduced as $\sim\frac{3k_{sp}\delta^2}{2}$, dividing it by the volume yields the strain energy density,

$$\Delta\Pi=\frac{3k_{sp}}{2}\left(\frac{\delta^2}{s_0^3}\right) \qquad (40.5)$$

The compression modulus can then be found by comparing 40.4 and 40.5 to obtain, $K_V=\frac{k_{sp}}{3s_0}$, showing that elastic moduli depend upon the spring constant and the spring length in the equilibrium condition.

Entropic networks

We will now consider the properties of a network of flexible chains which are packed to sufficient density that each chain is in proximity with its neighbours at several locations along its contour length. A cross-linker is then added to this assembly of chains which weld each chain to its neighbour at several random locations. In this process, the network becomes cross-linked; it no longer remains fluidic but attains a rigidity, the extent of which depends upon the density of the cross-linking nodes. Question arises how this network of chain behaves when subjected to external stress. In fact, after crosslinking, each chain segment between the cross-linking nodes in essence behaves like a random chain and its end to end displacement $\overline{r_{ee}}$ obey the Gausian probability distribution as discussed earlier. As a result, the contour length of the chain remains unaltered, however the location of the crosslinking nodes does not remain fixed in space at a non-zero temperature; the instantaneous end to end displacement varies. The average value of $\overline{r_{ee}}$ changes also when the network is subjected to external stresses. In this section we will like to deduce quantitatively how exactly this change occurs.

Let us consider that the system is in the shape of a rectangular prism of initial length L_x, L_y, L_z, which when deforms result in a prism of length $\wedge_x L_x, \wedge_y L_y, \wedge_z L_z$, such that the scaling factors or the extension ratios are greater than 1, $\wedge > 1$ for extension but smaller than 1, $\wedge < 1$ for compression. Question is how the entropy of the system changes with the factor $\wedge$.

After this deformation occurs, the probability that a given chain has a particular end to end displacement vector, $\overline{r_i} = r_i(x_i, y_i, z_i)$ is obtained considering that it has a displacement vector $(x_i/\wedge_x, y_i/\wedge_y, z_i/\wedge_z)$ in the unstressed state but has a displacement vector (x_i, y_i, z_i) after deformation. What is the probability that the displacement vector of the chain lies within the range $\overline{r_i}$ to $\overline{r_i + \Delta r}$ after deformation.

This probability is written as $\wp(x_i/\wedge_x, y_i/\wedge_y, z_i/\wedge_z) \cdot (\Delta x/\wedge_x) \cdot (\Delta y/\wedge_y) \cdot (\Delta z/\wedge_z)$, where,

$$\wp(x_i, y_i, z_i) = (2\pi\sigma^2)^{-3/2} \exp\left(-\frac{x^2 + y^2 + z^2}{2\sigma^2}\right)$$

is the three dimensional probability density function as derived earlier. Here, for a three dimensional chain of N equal segments of length b, $\sigma^2 = \frac{Nb^2}{3}$ (equation 37.15). Using the above relation we can obtain the probability that a chain lies within the above volume element is,

$$\eta_i = (2\pi\sigma^2)^{-3/2} \exp\left\{-\frac{(x_i/\wedge_x)^2 + (y_i/\wedge_y)^2 + (z_i/\wedge_z)^2}{2\sigma^2}\right\} \frac{\Delta x \Delta y \Delta z}{\wedge_x \wedge_y \wedge_z} \qquad (40.6)$$

Entropic networks (contd...)

But the question is how many of the n individual segments have number of chains n_i for each range $\overline{r_i}$. We can choose n_i out of n in $n!/\Pi_i n_i!$ number of ways. The probability that any one of these configurations will have the end to end displacement $\overline{r_i}$ is given by the above relation for η_i in equation 40.6. Hence the probability that all of the configurations will have the end to end displacement $\overline{r_i}$ is given as,

$$\wp_a = \left(\Pi_i \eta_i^{n_i}\right)\cdot\left(n!/\Pi_i n_i!\right) = n!\Pi_i\left(\eta_i^{n_i}/n_i!\right) \qquad (40.7)$$

We need to find out also the probability that each cross-linking site lies within an appropriate distance, essentially within a volume element δV of a site of a neighbouring chain in order that the crosslinking happens. An estimate of this probability can be written as,

$$\wp_b = (n/2)!\left(2\delta V/V\right)^{n/2} \qquad (40.8)$$

So the probability that a network has a particular configuration after deformation is the product of above two probabilities, i.e. $\wp_a \wp_b$. The corresponding entropy of the network is written as $S = k_B \ln \wp_a + k_B \ln \wp_b$, where k_B is the Boltzman constant. Expanding for the expression for $\wp_a$ and $\wp_b$, and simplifying, the expression of entropy is obtained as,

$$S = -(k_B n/2)\left[\wedge_x^2 + \wedge_y^2 + \wedge_z^2 - 3 - \ln \wedge_x \wedge_y \wedge_z - \ln(n/2)! - (n/2)\ln\left(2\delta V/V_0\right)\right] \qquad (40.9)$$

Hence the change in entropy from the reference state of unstretched configuration: $\wedge_x = \wedge_y = \wedge_z = 1$, is

$$\Delta S = -(k_B n/2)\left[\wedge_x^2 + \wedge_y^2 + \wedge_z^2 - 3 - \ln \wedge_x \wedge_y \wedge_z\right] \qquad (40.10)$$

Hence the free energy change is obtained as $\Delta F = -T\Delta S$

$$\Delta F = (k_B T n/2)\left[\wedge_x^2 + \wedge_y^2 + \wedge_z^2 - 3 - \ln\left(\wedge_x \wedge_y \wedge_z\right)\right] \qquad (40.11)$$

Considering that volume conservation requires $\wedge_x \wedge_y \wedge_z = 1$, we have

$$\Delta F = (k_B T n/2)\left[\wedge_x^2 + \wedge_y^2 + \wedge_z^2 - 3\right] \qquad (40.12)$$

For pure shear $\wedge_x = \wedge = 1/\wedge_y$ and $\wedge_z = 1$, so that the expression for free energy simplifies to

$$\Delta F = (k_B T n/2)\left[\wedge^2 + 1/\wedge^2 - 2\right] = (k_B T n/2)\left[\wedge - 1/\wedge\right]^2 \qquad (40.13)$$

Putting $\wedge = 1+\delta$ and considering that δ is small, the change in free energy is obtained as $\Delta F = (k_B T n/2)4\delta^2$. Dividing this expression by undeformed volume V_0 we obtain,

$$\Delta F = 2\delta^2 \rho k_B T \qquad (40.14)$$

Where is the density of chains. From 40.1 for pure shear conditions, , such that

$\rho = n/V_0$ $\qquad\qquad$ $\wedge = 1 + \delta$

$u_{xx} = \delta$, $u_{yy} = -\delta$ and $u_{zz} = 0$ we obtain

$$\Delta F = 2\delta^2 \mu \qquad (40.15)$$

Comparing equation 40.14 and 40.15, the shear modulus of the network is obtained as

$$\mu = \rho k_B T \qquad (40.15)$$

Computer simulation of networks confirms the density dependence of the shear modulus as derived above.

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Summary and future directions:

The objective of this course was to show how one can use well developed theoretical tools of mechanics in analyzing variety of problems related to soft deformable materials, e.g. indentation of a block of gel, separation of adhered surfaces, bending of thin plates and sheets, bending and torsion of rods and so on. We touched upon also the emerging areas of soft mechanics in elasto-capillary effect, mechanics of networks, elasticity of sub-cellular filaments. Through these discussions we have shown that basic principles in elasticity can be implemented in the context of large variety of problems which can enhance our understanding of various natural phenomena. There tools will be useful also in understanding several other problems in these areas.

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