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Remarks on "Poisson Ratio beyond the Limits of the Elasticity Theory"

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Generalizing the discussion presented for the three-dimensional case in the textbook by Landau and Lifshitz,[1)] one can write the free energy of an elastic deformation described by the (Lagrange) strain, ε_{ij}, in a D-dimensional isotropic medium, which was at zero external stress before the deformation, as the sum of the second order invariants obtained from the strain components

$$F_{\text{elast}} = \frac{\lambda}{2}\varepsilon_{ii}^2 + \mu\varepsilon_{ij}^2, \tag{1}$$

where the general summation rule on repeated indices is used.[1)] The quantities λ, μ are called *Lamé coefficients*.[1)]

To obtain stability conditions of the isotropic medium, it is convenient to use decomposition of the strain into hydrostatic compression and pure shear.[1)] The formula (1) is then replaced by

$$F_{\text{elast}} = \frac{K}{2}\varepsilon_{ll}^2 + \mu\left(\varepsilon_{ij} - \frac{1}{D}\delta_{ij}\varepsilon_{ll}\right)^2, \tag{2}$$

where δ_{ij} is the Kronecker delta, and

$$K = \lambda + \frac{2\mu}{D}. \tag{3}$$

The quantities K, μ are called the bulk modulus and the shear modulus, respectively, and, as is well known,[1)] the quadratic form (2) is positive definite if and only if they are positive. Thus, the relations

$$K > 0, \quad \mu > 0 \tag{4}$$

are necessary and sufficient for the stability of the considered D-dimensional isotropic medium.

The Poisson ratio, σ, is defined as the negative ratio of the strain, ε_{yy}, in the (transverse) direction y perpendicular to the direction x in which an infinitesimal change of stress has been applied, to the change of the strain, ε_{xx}, in the (longitudinal) direction x in which the stress has been changed.

Following the well known arguments, described for the three dimensional case in the textbook by Landau and Lifshitz,[1)] one obtains the expression for σ in the D-dimensional isotropic medium

$$\sigma = \frac{DK - 2\mu}{(D-1)DK + 2\mu}$$

$$= \frac{\lambda}{(D-1)\lambda + 2\mu}. \tag{5}$$

Taking into account the stability conditions (4) and the first of the above equalities, one obtains the limits for the Poisson ratio of a D-dimensional isotropic medium

$$-1 \le \sigma \le \frac{1}{D-1}. \tag{6}$$

From the second equality in (5) one concludes that when the isotropic medium is stable the Poisson ratio is positive, $\sigma > 0$, if and only if the first Lamé coefficient is positive, $\lambda > 0$. So, if the stability conditions had been such as claimed in ref. 2 (i.e. positive Lamé coefficients, $\lambda > 0$, $\mu > 0$) then negative Poisson ratios would never occur. It is well known, however, that the Poisson ratio *can* be negative and, hence, it is *not* necessary for λ to be positive. This is in clear contradiction with the first sentence of ref. 2.

Substituting $D = 3$ for a three-dimensional (3D) isotropic medium one obtains the Poisson ratio limits mentioned in the second sentence of ref. 2

$$-1 \le \sigma \le \frac{1}{2}. \tag{7}$$

These limits, however, are correct only for 3D systems. For any isotropic two-dimensional system (2D) the correct limits for the Poisson ratio are

$$-1 \le \sigma \equiv \frac{K-\mu}{K+\mu} \le 1. \tag{8}$$

Although in ref. 2 the Authors consider a 2D system which is anisotropic, in general, they concentrate on two aspects related to *isotropic* systems: (i) a single point, $\sigma_x = \sigma_y = 1$, and (ii) possible isotropic structures formed by random 'polycrystalline' system. In the context of the condition (8) it is neither surprising nor in conflict with conventional elasticity theory that the Poisson ratios σ_x, σ_y reach at the same time the value unity for the 2D model. It is also neither surprising nor in conflict with conventional elasticity theory that one can obtain 2D polycrystals with $\sigma > 1/2$.

However, contrary to the claims in ref. 2, the relation (7) has to be fulfilled by *any* 3D isotropic medium, no matter if in the framework of the conventional elasticity theory[1)] or in the framework of Cosserat elasticity,[3)] which takes micro-rotations into account.

In the conclusions of ref. 2 the Authors claim that two factors are important to obtain large σ: anisotropy and the deformation due to rotation of microscopic clusters. Neither of these factors is necessary, however. As it was not specified in ref. 2 whether the anisotropy was related to the structure or to the particles, both these possibilities are considered in the examples below. Because of the limited space available, only periodic structures will be considered as they can be easily solved exactly, what simplifies the discussion.

In Fig. 1 a simple model system of 2D cyclic trimers is presented. Although this system does not show any infinite-fold symmetry axis (which, for obvious reasons, cannot occur in any ordered periodic structure), it is *elastically isotropic* by the symmetry of the model. This is because (at

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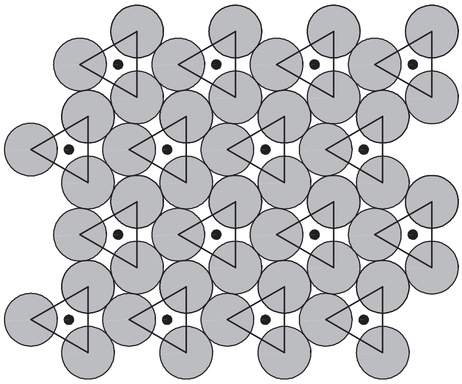

Fig. 1. The non-chiral, elastically isotropic model exhibiting Poisson ratio in the range $-1 \le \sigma \le 1$ *without* any molecular rotation. The centers of the discs-atoms (represented by the circles of diameter b) are placed in the vertices of a perfect triangle of the side length equal to σ.

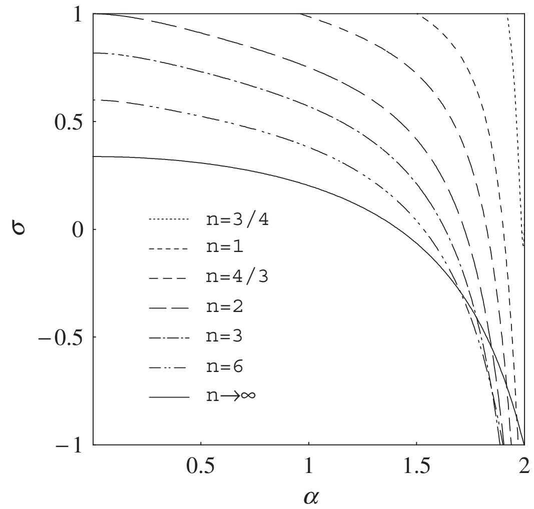

Fig. 2. The Poisson ratio of the mechanically stable (K, $\mu > 0$) structure shown in Fig. 1 as a function of the dimensionless inverse distance between the nearest-neighboring atoms of different molecules, $\alpha = \sigma b^{-1}$, for the n-inverse-power interaction, $u(r) = u_1(r/\sigma)^{-n}$, between all pairs of atoms belonging to neighboring molecules. The values of the power n are shown in the figure. The number density in the system is equal to $N/V = \frac{8}{\sqrt{3}}[(\sqrt{3} + \sqrt{4\alpha^{-2} - 1})\sigma]^{-2}$.

small deformations) the elastic properties of any 2D system exhibiting a three-fold symmetry axis do not depend on the direction. Namely, the three-fold axis implies that the fourth-rank tensor of the elastic constants is isotropic and the second order expansion of the system free energy in the strain tensor components has the form given by the formula (1); this can be proven in the way analogous to that described in the case of the six-fold axis.[1)] (It is worth to add that this "symmetry mechanism" in two dimensions implies that the system is elastically isotropic for *any* interaction potential and *any* size of the unit cell for which the system is stable at given thermodynamic conditions. This is in contrast to the 3D systems, for which no periodic lattice is elastically isotropic by the symmetry alone,[1)] and for which the only way to obtain a crystal whose elastic properties are direction independent is by applying the "energetic mechanism" in the form of various conditions imposed on the interaction potential.) Though the molecules of the model system in Fig. 1 do *not* exhibit any rotation, it can be seen in Fig. 2 that the Poisson ratio of this system can be varied from -1 to 1 by changing the density. It should be stressed that, in general, the system shown in Fig. 1 can be subject to non-zero external pressure, i.e. linear terms in the strain tensor components can appear in the expansion (1). Thus, *effective* shear and bulk moduli are required, in general. The details of this approach can be found, *e.g.*, in an earlier work of the present Author[4)] where another elastically isotropic model (being, however, chiral) has been described, which can also show positive Poisson ratio exceeding 1/2 without any molecular rotation [see Figs. 1(b), (c) in ref. 4]. Moreover, a Poisson ratio exceeding 1/2 can be also obtained for elastically isotropic lattices in 2D even for *isotropic* intermolecular interactions.[5)]

The following conclusions result from the discussion above:

(1) the positive sign of the Lamé constant λ is not necessary for the stability of an isotropic system at any dimensionality,
(2) as the upper limit for the Poisson ratio in 2D isotropic systems is 1, it is not surprising that crystalline or polycrystalline 2D systems can be obtained having the Poisson ratio exceeding 1/2,
(3) both the traditional theory of elasticity and the Cosserat theory exclude Poisson ratios exceeding 1/2 in 3D isotropic systems,
(4) neither anisotropy nor rotation are necessary to obtain extreme values of the Poisson ratio.[4–7)]

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