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THE MATHEMATICAL MODEL FOR ANISOTROPIC MATERIAL WITH AUXETIC PROPERTIES

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Abstract. A two-dimensional model representing a square lattice of round particles is proposed for description of auxetic properties of an anisotropic crystalline material with cubic symmetry. It is assumed that each particle has two translational and one rotational degrees of freedom. Differential equations describing the propagation of elastic and rotational waves in such a medium have been derived. Relationships between the macroelasticity constants of the medium and the parameters of its inner structure have been found. It has been shown that the Poisson's ratios of the anisotropic material can be negative for certain values of the parameters of its inner structure.

1. Introduction

One of the most important characteristics of elasticity of a material is the Poisson's ratio ν, which is a relation of transverse compression to elongation in the case of a pure tension. From the classical theory of elasticity it is known that theoretically justified values of the Poisson's ratio lie in the range $-1 \le \nu \le 0{,}5$ [1]. The upper limit corresponds to incompressible materials (particularly, rubber), which save their volume during deformation, but their shape changes substantially. The lower limit corresponds to materials, which geometric proportions are constant during deformation, but their volume varies. Materials with negative Poisson's ratio are of special interest. Porous media, granular materials, polymers, composites, and crystalline media are good examples of such materials [1, 2]. The first reliable mention of the experimentally observed negative values of Poisson's ratio (quartz crystals at high temperatures) refers to 1962 [3]. At present, a term *auxetics* (from the Greek "auxetos" - "swelling") is widely used for these materials. This term was proposed by K. Evans in 1991 [4]. Nowadays, in the scientific literature there appear rather many publications about porous materials and nanomaterials possessing auxetic properties (see, for example, [5, 6]). Advantages of these materials are their high consumer values (low density, good insulation properties, etc.). However, description of auxetic properties is impossible without a mathematical model. Within the scope of the classical theory of elasticity that considers a medium as a continuum of material points such description is very problematic. For this reason, modelling necessitates to represent a medium by a regular or quasi-regular lattice, the sites of which are occupied by small-size bodies possessing additional degrees of freedom (rather than material points). Domains, granules, fullerenes, nanotubes, or clusters of nanoparticles can play the role of such bodies. As a rule, two-dimensional models are currently used for media with auxetic properties, but in such models there is a rather complex system of connections between the anisotropic particles, in particular, which can be squares (see, for example, [1, 7]).

In this paper, a two-dimensional dynamic model for an anisotropic material is elaborated that represents a square lattice, sites of which are occupied by the non-deformable particles with two translational and one rotational degrees of freedom, and the space between the particles is a massless elastic medium, through which the force and moment interactions are transmitted. As it will be shown below, the Poisson's ratios of such a material can be negative for some values of the parameters of its inner structure.

2. The mathematical model for an anisotropic medium

In an anisotropic monocrystalline material with a cubic lattice the Poisson’s ratios in special crystallographic directions <100>, <110>, and <111> are found by known relations [8]:

$$\nu_{<100,001>} = \frac{C_{12}}{C_{11}+C_{12}}, \quad \nu_{<110,001>} = \frac{4C_{12}C_{44}}{2C_{11}C_{44}+(C_{11}-C_{12})(C_{11}+2C_{12})}, \tag{1}$$

$$\nu_{<110,1\bar{1}0>} = \frac{(C_{11}-C_{12})(C_{11}+2C_{12})-2C_{11}C_{44}}{(C_{11}-C_{12})(C_{11}+2C_{12})+2C_{11}C_{44}}, \quad \nu_{<111,111>} = \frac{C_{11}+2C_{12}-2C_{44}}{2(C_{11}+2C_{12}+C_{44})}, \tag{2}$$

where C_{11}, C_{12}, and C_{44} are the elasticity constants of the second order, which are coefficients of the classical Lame equations for media with cubic symmetry, and all of them are contained even in the two-dimensional analog of these equations:

$$\rho u_{tt} = C_{11}u_{xx} + C_{44}u_{yy} + \left(C_{12}+C_{44}\right)w_{xy},$$

$$\rho w_{tt} = C_{44}w_{xx} + C_{11}w_{yy} + \left(C_{12}+C_{44}\right)u_{xy}, \tag{3}$$

where ρ is the density of a medium with cubic symmetry. Obviously, if the Poisson's ratios (1) are always greater than zero for positive elasticity constants, then the Poisson's ratios (2) can take on negative values. For adequate description of the physical and mechanical properties of an auxetic material, a mathematical model will be elaborated that enables one to relate the elasticity constants, and hence, due to Eqs. (1) and (2), the Poisson's ratios, to the microstructure parameters of such a material.

The model representing a square lattice (Fig. 1), the sites of which are occupied by the homogeneous round particles (granules) with diameter d and mass M, will be considered below. In the initial state, the mass centres of the particles are located in the lattice sites N that are enumerated using couple of indices (i, j), and the distance between the neighbouring particles equals a. Only small deviations of the particles from the equilibrium states are considered and it is assumed that each particle has three degrees of freedom: the mass centre displacements $u_{ij}(t)$ and $w_{ij}(t)$, respectively, along the x- and y-axes and the rotation $\phi_{ij}(t)$ with respect to the axis passing through the mass centre of the particle (Fig. 2). The particle N is supposed to interact directly with eight nearest neighbours in the lattice. The mass centers of first four of them are located at distance a from the particle N (these are *particles of the first coordination sphere*). The mass centres of remaining four neighbours are situated on diagonals of the square lattice (*particles of the second coordination sphere*). These interactions are modelled by elastic springs of three types. The central springs with rigidity K_1 describe interactions between the granules at extension/compression of the material. The diagonal springs with rigidity K_2 characterize force interactions of the particles of shear deformation in the material. And, at last, the springs K_3 simulate interactions of the central particle with granules of the second coordination sphere. For convenience of calculations it is assumed that the connection points of the springs K_1 lie in the centres of round particles, whereas the connection points of the springs K_2 and K_3 coincide with the vertices of the square with side $h = d/\sqrt{2}$ that is entered in a circumference (Fig. 2).

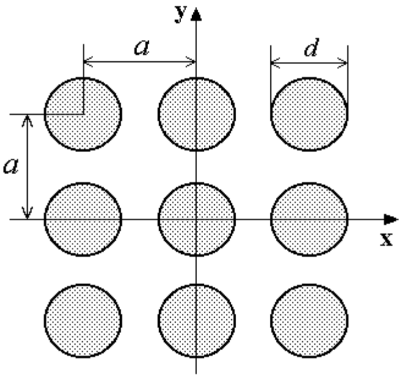


Fig. 1. The square lattice consisting of round particles.

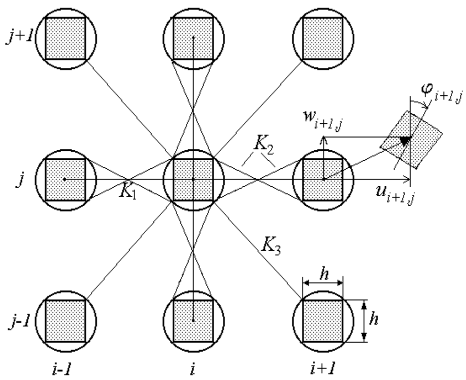


Fig. 2. The scheme of force interactions and kinematics of the particles.

Under these assumptions, the dynamics of the considered medium is described in the continuum approximation by the following equations [9-11]:

$$u_{tt} - c_1^2 u_{xx} - c_2^2 u_{yy} - s^2 w_{xy} + \beta^2 \phi_y = 0,$$

$$w_{tt} - c_2^2 w_{xx} - c_1^2 w_{yy} - s^2 u_{xy} - \beta^2 \phi_x = 0,$$

$$\phi_{tt} - c_3^2(\phi_{xx} + \phi_{yy}) + \beta^2 R^{-2}(2\phi + w_x - u_y) = 0. \quad (4)$$

Here, the following notation has been introduced: c_1, c_2, and c_3 are the velocities of propagation of longitudinal, transverse, and rotational waves, respectively, s is the coefficient of linear coupling between the longitudinal and transverse waves, β is the parameter of coupling of microrotations with the transverse and longitudinal waves, and $R = d/\sqrt{8}$ is the radius of the mass moment of inertia of the particle.

Dependences of coefficients of equations (4) on microstructure parameters (size of particles d, lattice period a, and parameters of force interactions K_1, K_2 and K_3) have the following form:

$$\rho c_1^2 = \frac{K_1}{a} + \frac{2(a\sqrt{2}-d)^2}{d^2 + (a\sqrt{2}-d)^2}\frac{K_2}{a} + \frac{K_3}{a}, \quad \rho c_2^2 = \frac{2d^2}{d^2 + (a\sqrt{2}-d)^2}\frac{K_2}{a} + \frac{K_3}{a},$$

$$\rho c_2^2 = \frac{2d^2}{d^2 + (a\sqrt{2}-d)^2}\frac{K_2}{a} + \frac{K_3}{a}, \quad \rho\beta^2 = \frac{2d^2}{d^2 + (a\sqrt{2}-d)^2}\frac{K_2}{a} = \rho\left(c_2^2 - \frac{s^2}{2}\right). \quad (5)$$

For comparison of the set (4) with the classical equations (3) it is necessary to pass into approximation of the second-order gradient theory of elasticity. In this case equations (4) take on the form [10-11]:

$$u_{tt} - c_1^2 u_{xx} - (c_2^2 - \frac{\beta^2}{2})u_{yy} - (s^2 + \frac{\beta^2}{2})w_{xy} = \frac{R^2}{4}\frac{\partial}{\partial y}\left[\frac{\partial^2}{\partial t^2}\left(u_y - w_x\right) - c_3^2 \Delta\left(u_y - w_x\right)\right],$$

$$w_{tt} - (c_2^2 - \frac{\beta^2}{2})w_{xx} - c_1^2 w_{yy} - (s^2 + \frac{\beta^2}{2})u_{xy} = -\frac{R^2}{4}\frac{\partial}{\partial x}\left[\frac{\partial^2}{\partial t^2}\left(u_y - w_x\right) - c_3^2 \Delta\left(u_y - w_x\right)\right]. \quad (6)$$

Here symbol Δ denotes a two-dimensional Laplacian $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$.

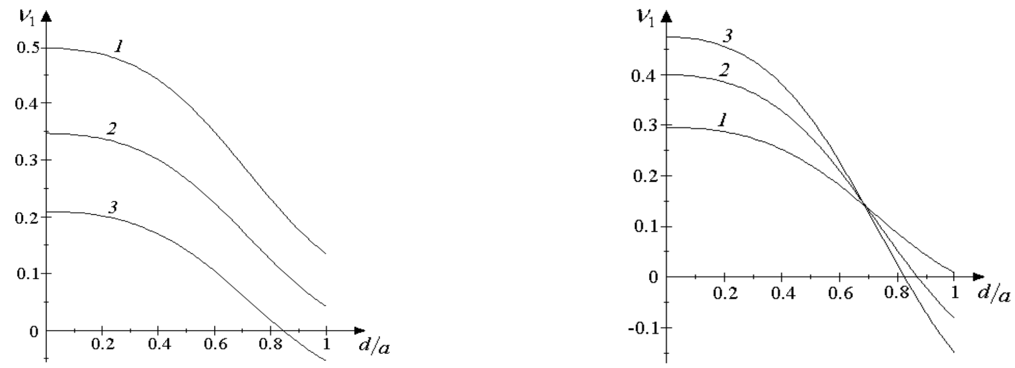
From comparison of equations (3) with the left-hand sides of equations (6) it follows that

$$C_{11} = \rho c_1^2, \quad C_{12} = \rho s^2/2, \quad C_{44} = \rho(2c_2^2 + s^2)/4. \tag{7}$$

Then, using relationships (7) and (5) it is possible to obtain the following dependences of the elasticity constants of the second order on the microstructure parameters:

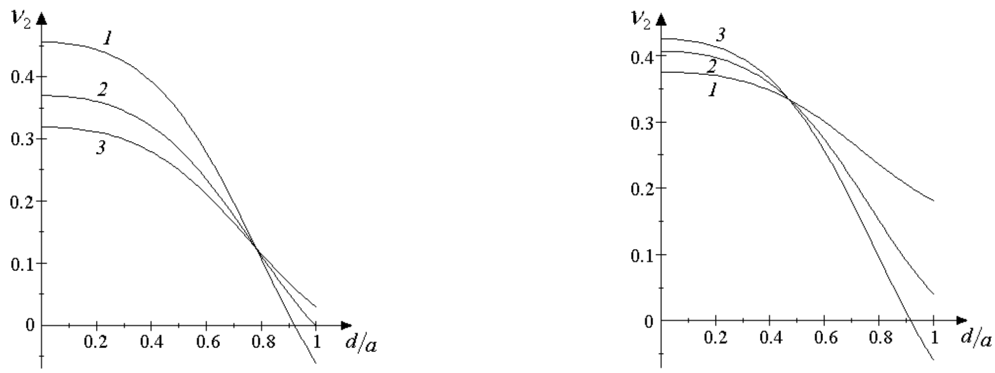
$$C_{11} = \frac{K_1 + K_3}{a} + \frac{2(a\sqrt{2}-d)^2}{d^2 + (a\sqrt{2}-d)^2}\frac{K_2}{a}, \quad C_{12} = \frac{K_3}{a}, \quad C_{44} = \frac{d^2}{d^2 + (a\sqrt{2}-d)^2}\frac{K_2}{a} + \frac{K_3}{a}. \tag{8}$$

Substitution of expressions (8) into formulas (2) gives a possibility to analyze influence of the medium microstructure on the corresponding anisotropic Poisson's ratios. Dependences of the Poisson's ratios $\nu_1 = \nu_{<110,1\bar{1}0>}$ and $\nu_2 = \nu_{<111,111>}$ on the relative size of the particles d/a are plotted for various values of the parameters of force interactions K_2/K_1 and K_3/K_1 in Figs. 3 and 4. From these figures it is visible that negative values of ν_1 and ν_2 are provided, basically, by large size of the particles: $d/a \to 1$. However, if $\nu_2 < 0$ only for $K_2 >> K_3$, then $\nu_1 < 0$ for different relations between K_2/K_1 and K_3/K_1.



a) b)

Fig. 3. Dependences of the Poisson's ratio $\nu_1 = \nu_{<110,1\bar{1}0>}$ on the relative size of the particles for $K_3/K_1 = 0.37$ (curve 1), 0.6 (curve 2), 0.9 (curve 3), $K_2/K_1 = 0.3$ (a) and for $K_2/K_1 = 0.3$ (curve 1), 0.6 (curve 2), 0.9 (curve 3), $K_3/K_1 = 0.7$ (b).



a) b)

Fig. 4. Dependences of the Poisson's ratio $\nu_2 = \nu_{<111,111>}$ on the relative size of the particles for $K_3/K_1 = 0.1$ (curve 1), 0.4 (curve 2), 0.7 (curve 3), $K_2/K_1 = 1$ (a) and for $K_2/K_1 = 0.3$ (curve 1), 0.7 (curve 2), 1.1 (curve 3), $K_3/K_1 = 0.2$ (b).

3. Conclusions

A two-dimensional model for a crystalline material with a cubic lattice has been elaborated. The correlation between the elasticity constants of such a medium and its microstructure parameters has been revealed. The anisotropic Poisson's ratios are shown to be negative for certain values of the microstructure parameters, that is in a good agreement with the known experimental data [6, 8].

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