INTERPARTICLE INTERACTION IN A DEFORMED BODY. II. THEORY OF ELASTICITY FOR A BODY OF THE NTH COORDINATION ORDER

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In the framework of the model of structurally continual media described in the first part of the work [Mat. Sci., 33, No. 2, 125-134 (1997)], we construct the theory of elasticity for an anisotropic body of the n-th coordination order by using the thermodynamic approach. Unlike the classical theory of elasticity for anisotropic bodies, in the constructed theory, the role of bulk forces is played by the forces of interparticle interaction. We introduce matrices of new material constants which characterize the nano-mechanical properties of the body from the macroscopic point of view and describe the field of natural elastic waves of a given anisotropic structurally continual medium.

The present work is devoted to the mathematical simulation of the influence of interparticle interaction on the stress-strain state of a solid body with regular structure.

The mathematical description of the forces of interparticle interaction in elastic anisotropic bodies of the n-th coordination order [1] is performed within the framework of the thermodynamic approach [2, 3]. As the function of state at constant temperature, we take the internal energy of the body which has the form of a sum of two independent components, namely, of the strain energy and potential energy of interparticle interaction. These components represent two different nanophysical aspects of the same mechanical process. As independent degrees of freedom for a body of this sort, we use transverse (simple shear) and longitudinal (variations of the distance) relative displacements of its material points as well as the collection of deformational degrees of freedom corresponding to the variation of the volume and shape of the body, i.e., to tensile (compressive) and shear strains. Parallel with the existing constants of the mechanics of deformable body, we introduce matrices of new material constants which characterize the nanoscopic properties of the body on the level of mechanical analysis of the n-th coordination order. We assume that stresses induce the deformation of the body, the appearance of nonzero elastic displacements, and an increment of generalized forces of interparticle interaction identified with bulk forces. The law of conservation of momentum for an arbitrary volume is written in the form of a generalized equation of motion in terms of displacements. The analysis of the stress-strain state of an anisotropic body of the n-th coordination order is reduced to the formulation of basic boundary-value problems.

Internal State of the Body

Assume that the body \( D^p \) is a monocrystal and, together with an ambient medium, represents a thermodynamic system (in a macrophysical sense) [2–4]. In the framework of this system, one can express all quantitative laws via the parameters of the monocrystal and exclude the characteristics of the medium from consideration. In view of this, we equip the body \( D^p \) with the following properties:

The body \( D^p \) occupies a volume \( V^p \) bounded by the surface \( \partial D^p \). We equip it with a single principal value of the natural frequency \( \omega_n \) (\( \omega_n^2 = \omega_n^t = \omega_n^s \)) (its coordination order is related to the shear lattice \( C^{n} \) [1]) and two families of degrees of freedom. The first family consists of two independent subsets, namely, of a subset of elastic displacements connected with changes (increase and decrease) in the distances between particles and a subset of simple shear of material points (we do not consider rigid linear displacements and rotations of the material points as a rigid body). We describe these subsets by the vectors \( \vec{u}_m^\gamma \) with components \( u_m^\gamma \) (\( \gamma = d, s, \ m = 1, 2, 3 \)).
are continuous functions of three Cartesian coordinates \( x_1, x_2, \) and \( x_3 \) and time \( \tau \), i.e., \( u_i^m = u_i^m(x_1, x_2, x_3, \tau) = u_i^m(\vec{r}, \tau) \), where \( \vec{r} \) is the radius vector of a material point of the body (relation (1) in [1]). The first and second partial derivatives of the functions \( u_i^m \) with respect to \( x_1, x_2, x_3, \) and \( \tau \) exist and are continuous. Moreover, the vectors of elastic displacements of increase and decrease in the distance \( (\vec{u}^{dn}) \) and shear \( (\vec{u}^{sn}) \) for two neighboring material points are parallel to the vectors of the relevant total displacements of these points. However, \( \vec{u}^{dn} \) is a potential vector and \( \vec{u}^{sn} \) is a vector of a vortex field. This means that the vectors of elastic displacements of increase and decrease in the distance \( (\vec{u}^{dn}) \) and shear \( (\vec{u}^{sn}) \) must satisfy the relations

\[
\text{rot} \vec{u}^{dn} = \vec{0} \quad \text{and} \quad \text{div} \vec{u}^{sn} = 0,
\]

where \( \vec{0} \) is a vector of length zero.

On the macrolevel of mechanical analysis, elastic displacements of increase and decrease in the distance \( (u^{dn}_m) \) and shear \( (u^{sn}_m) \) for any material point of the body reproduce the macroscopic influence of surrounding material points on this point as well as the action of the indicated point upon surrounding points.

Since the displacements \( u^{dn}_m \) and \( u^{sn}_m \) are linear, we have

\[
u^{dn}_m + u^{sn}_m = u^m_m,
\]

where \( u^m_m \) are generalized displacements which are the components of the vector sum \( (\vec{u}^n) \) of elastic displacements of increase and decrease in the distance \( (\vec{u}^{dn}) \) and shear \( (\vec{u}^{sn}) \).

The second family of degrees of freedom depends on the deformational properties of the material and is described by the components \( e^m_{ml} \) of the symmetric strain tensor \( \{e^m_{ml}\} \) \( (m, l = 1, 3) \). The deformations \( e^m_{ml} \) are expressed via generalized displacements \( u^m_m \) (2) by the Cauchy relations

\[
e^m_{ml} = \frac{1}{2} (u^m_{l,m} + u^m_{m,l}),
\]

where the commas placed in subscripts denote the operation of differentiation with respect to the relevant variable, i.e.,

\[
\vec{l} = \frac{\partial}{\partial x_i}.
\]

We now consider the case where the body is not mechanically isolated. This means that, in the process of interaction with external mechanical factors, elastic waves propagate from one nanoparticle to another carrying phonons from the surface into the bulk of the body. This kind of energy transfer is accompanied by the excitation of natural oscillations with natural frequency \( \omega_n \) as well as by mutual displacements of nanoparticles and results in the violation of thermodynamic equilibrium in every elementary local volume \( \partial V^p \). The body is deformed and the forces of interparticle interaction acquire certain increments spent for the mechanical work \( A \) of transition to a new state of local thermodynamic equilibrium of the body and in the process of interaction with external mechanical factors. This process terminates as soon as the state of thermodynamic equilibrium is attained in every elementary local volume \( \partial V^p \), i.e., after the transformation of traveling elastic waves into standing waves.

The amount of work \( A \) [3] depends on the macrophysical aspects of mechanical processes running in the body, in particular, on its deformation and interparticle interactions (the presence of internal friction is neglected). We assume that the process of deformation of the body is independent of the process of interparticle interactions. In the thermodynamic space, each macrophysical component of mechanical processes is associated with its own pair of sets of parameters of state of the body \( D^p \) [3].