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Abstract

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THEORY OF ELASTICITY

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COMPUTATION OF ELASTIC CONSTANTS FROM MICROSCOPIC QUANTITIES FOR AN ELASTIC MEDIUM WHOSE ENERGY DEPENDS ON STRAIN GRADIENTS

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In a number of works (see, for example, ⁽¹⁻⁴⁾) a generalized theory of elasticity is considered in which the elastic energy is represented in the form of a quadratic form in the strains and the strain gradients with respect to the coordinates. In the classical theory of elasticity the density of elastic energy U is represented in the form

$$U = 1/2 c^{iklm} \varepsilon_{ik} \varepsilon_{lm}, \quad (1)$$

where the elastic constants c^{iklm} can be expressed in terms of the force constants of the crystal lattice. In the present work formulas are obtained which express the coefficients of the quadratic form of the elastic-energy density in the generalized theory of elasticity in terms of the force constants of the crystal lattice.

In passing from the micromodel to the continuum we shall use the method developed in ^(5,6). As the initial micromodel we take the Born model of a simple crystal lattice in the harmonic approximation ⁽⁷⁾. The potential energy of the lattice is taken in the form

$$\Phi = 1/2 \sum_{n,n'} u_{\alpha}(n) \Phi^{\alpha\beta}(n-n') u_{\beta}(n'), \quad (2)$$

where $n = n^{\alpha} e_{\alpha}$ is a vector in an oblique lattice coordinate system with basis e_{α} (the lattice sites correspond to integral components n^{α}), $u(n)$ are the displacements of the particles, and $\Phi^{\alpha\beta}(n-n')$ are the force constants.

It was shown in ^(5,6) that, by means of a certain interpolation, one can pass from functions of the discrete argument n to analytic functions of x , with $\Phi^{\alpha\beta}(n)$ replaced by the function $\Phi^{\alpha\beta}(x)$, whose Fourier transform is

$$\Phi^{\alpha\beta}(k) = \frac{1}{V_A} \sum_n \Phi^{\alpha\beta}(n) e^{in \cdot k}; \quad (3)$$

here V_A is the volume of the elementary cell of the lattice. Then the potential energy Φ is written in the form

$$\begin{aligned} 2\Phi &= \iint u_\alpha(x) \Phi^{\alpha\beta}(x-x') u_\beta(x') dx dx' = \frac{1}{(2\pi)^3} \int \overline{u_\alpha}(k) \Phi^{\alpha\beta}(k) u_\beta(k) dk \\ &= \iint \varepsilon_{\nu\alpha}(x) c^{\nu\alpha\mu\beta}(x-x') \varepsilon_{\mu\beta}(x') dx dx' = \frac{1}{(2\pi)^3} \int \overline{\varepsilon_{\nu\alpha}}(k) c^{\nu\alpha\mu\beta}(k) \varepsilon_{\mu\beta}(k) dk, \end{aligned} \quad (4)$$

where $\varepsilon_{\nu\alpha}(x) = \partial_{(\nu} u_{\alpha)}(x)$ is the strain. Here a Fourier transformation with respect to x has been carried out.

The tensor $c^{\nu\alpha\mu\beta}$ is symmetric in the pairs $\nu\alpha$ and $\mu\beta$ and Hermitian with respect to interchange of the pairs.

It was shown in (5) that $\Phi^{\alpha\beta}(k)$ can be represented in the form

$$\Phi^{\alpha\beta}(k) = \psi^{\alpha\beta\nu\mu}(k) k_\nu k_\mu, \quad (5)$$

where the tensor $\psi^{\alpha\beta\nu\mu}$ is symmetric in $\nu\mu$ and Hermitian in $\alpha\beta$. The tensor $c^{\nu\alpha\mu\beta}(k)$ is constructed as follows

$$c^{\nu\alpha\mu\beta} = 1/2 (a^{\nu\alpha(\mu\beta)} + \overline{a^{\mu\beta(\nu\alpha)}}) + k_\lambda (a^{\nu\alpha\lambda(\mu\beta)} + \overline{a^{\mu\beta\lambda(\nu\alpha)}}), \quad (6)$$

here

$$a^{\nu\alpha\mu\beta}(k) = \psi^{\alpha\beta\nu\mu}(k) + \psi^{\nu\beta\alpha\mu}(k) - \psi^{\mu\beta\alpha\nu}(k), \quad (7)$$

$$a^{\nu\alpha[\mu\beta]}(k) = k_\lambda a^{\nu\alpha[\mu\beta]\lambda}(k),$$

the tensor $a^{\nu\alpha\mu\beta\lambda}$ being symmetric in $\nu\lambda$.

Represent $\psi^{\alpha\beta\nu\mu}(k)$ in the form

$$\psi^{\alpha\beta\nu\mu}(k) = \psi_0^{\alpha\beta\nu\mu} + k_\lambda \psi^{\alpha\beta\nu\mu\lambda}(k) \quad (8)$$

(here the subscript zero denotes the value of the function at $k = 0$). Then $a^{\nu\alpha\mu\beta}(k)$ can be represented in the form

$$a^{\nu\alpha\mu\beta}(k) = \psi_0^{\alpha\beta\nu\mu} + \psi_0^{\nu\beta\alpha\mu} - \psi_0^{\mu\beta\alpha\nu} + k_\lambda (\psi^{\alpha\beta\nu\mu\lambda}(k) + \psi^{\nu\beta\alpha\mu\lambda}(k) - \psi^{\mu\beta\alpha\nu\lambda}(k)) = a_0^{\nu\alpha\mu\beta} + k_\lambda a^{\nu\alpha\mu\beta\lambda}. \quad (9)$$

Substituting (7) and (9) into (6) and taking into account the symmetry properties of $\psi^{\alpha\beta\nu\mu}$, we obtain an expression for $c^{\nu\alpha\mu\beta}$ in terms of $\psi_0^{\alpha\beta\nu\mu}$ and $\psi^{\alpha\beta\nu\mu\lambda}(k)$:

$$c^{\nu\alpha\mu\beta}(k) = S_{0\chi\sigma\rho\tau}^{\nu\alpha\mu\beta} \psi_0^{\chi\sigma\rho\tau} + 1/4 k_\lambda [S_{1\chi\sigma\rho\tau}^{\nu\alpha\mu\beta} \psi^{\lambda\chi\sigma\rho\tau}(k) + S_{2\chi\sigma\rho\tau}^{\nu\alpha\mu\beta} \psi^{\chi\lambda\sigma\rho\tau}(k) + S_{3\chi\sigma\rho\tau}^{\nu\alpha\mu\beta} \psi^{\chi\sigma\rho\lambda\tau}(k)]. \quad (10)$$

Here the following symmetrization operators have been introduced:

$$S_{0\chi\sigma\rho\tau}^{\nu\alpha\mu\beta} = \delta_{\chi\sigma\rho\tau}^{\alpha\beta\nu\mu} + \delta_{\chi\sigma\rho\tau}^{\nu\beta\alpha\mu} - \delta_{\chi\sigma\rho\tau}^{\mu\beta\alpha\nu},$$

$$S_{1\chi\sigma\rho\tau}^{\nu\alpha\mu\beta} = \delta_{\chi\sigma\rho\tau}^{\nu\mu\beta\alpha} + \delta_{\chi\sigma\rho\tau}^{\alpha\beta\mu\nu} - 3\delta_{\chi\sigma\rho\tau}^{\beta\alpha\nu\mu} - 3\delta_{\chi\sigma\rho\tau}^{\mu\alpha\nu\beta},$$

$$S_{2\chi\sigma\rho\tau}^{\nu\alpha\mu\beta} = \delta_{\chi\sigma\rho\tau}^{\beta\mu\nu\alpha} + \delta_{\chi\sigma\rho\tau}^{\lambda\alpha\nu\beta} - 3\delta_{\chi\sigma\rho\tau}^{\alpha\nu\beta\mu} - 3\delta_{\chi\sigma\rho\tau}^{\nu\alpha\beta\mu},$$

$$S_{3\chi\sigma\rho\tau}^{\nu\alpha\mu\beta} = 4\delta_{\chi\sigma\rho\tau}^{\alpha\beta\nu\mu} + 4\delta_{\chi\sigma\rho\tau}^{\nu\beta\alpha\mu} + 4\delta_{\chi\sigma\rho\tau}^{\alpha\mu\nu\beta} + 4\delta_{\chi\sigma\rho\tau}^{\nu\mu\alpha\beta} - \delta_{\chi\sigma\rho\tau}^{\mu\beta\alpha\nu} - \delta_{\chi\sigma\rho\tau}^{\mu\alpha\alpha\nu} - \delta_{\chi\sigma\rho\tau}^{\alpha\nu\beta\mu} - \delta_{\chi\sigma\rho\tau}^{\nu\alpha\beta\mu},$$

where

$$\delta_{\chi\sigma\rho\tau}^{\alpha\beta\nu\mu} = \delta_\chi^\alpha \delta_\sigma^\beta \delta_\rho^\nu \delta_\tau^\mu.$$

Expand the analytic function $c^{\nu\alpha\mu\beta}(k)$ in a series in k :

$$c^{\nu\alpha\mu\beta}(k) = \sum_{p=0}^{\infty} c_p^{\nu\alpha\mu\beta\lambda_1 \dots \lambda_p} (-ik_{\lambda_1}) \dots (-ik_{\lambda_p}) \quad (11)$$

and carry out the same expansion under the integral sign in (4). Then the expression for the energy assumes the form:

$$2\Phi = \frac{1}{(2\pi)^3} \int \overline{\varepsilon_{\nu\alpha}(k)} c^{\nu\alpha\mu\beta}(k) \varepsilon_{\mu\beta}(k) dk = \frac{1}{(2\pi)^3} \int \overline{\varepsilon_{\nu\alpha}(k)} (c_0^{\nu\alpha\mu\beta} + c_1^{\nu\alpha\mu\beta\lambda_1} (-ik_{\lambda_1}) + c_2^{\nu\alpha\mu\beta\lambda_1\lambda_2} (-ik_{\lambda_1})(-ik_{\lambda_2}) + \dots)$$

For the density of elastic energy $\varphi(x)$ we obtain the expression

$$\varphi(x) = 1/2 (c_0^{\nu\alpha\mu\beta} \varepsilon_{\nu\alpha} \varepsilon_{\mu\beta} + c_1^{\nu\alpha\mu\beta\lambda_1} \varepsilon_{\nu\alpha} \partial_{\lambda_1} \varepsilon_{\mu\beta} + \dots)$$

$$\dots + (-1)^m c_{2m}^{\nu\alpha\mu\beta\lambda_1 \dots \lambda_{2m}} \partial_{\lambda_1} \dots \partial_{\lambda_m} \varepsilon_{\nu\alpha} \partial_{\lambda_{m+1}} \dots \partial_{\lambda_{2m}} \varepsilon_{\mu\beta} + \dots + (-1)^m c_{2m+1}^{\nu\alpha\mu\beta\lambda_1 \dots \lambda_{2m+1}} \partial_{\lambda_1} \dots \partial_{\lambda_m} \varepsilon_{\nu\alpha} \partial_{\lambda_{m+1}} \dots \partial_{\lambda_{2m+1}} \varepsilon_{\mu\beta} + \dots$$

Let us expand the functions $\psi^{\nu\alpha\mu\beta\lambda}$ in (10) also in a series in k . Taking (3), (5), (8), and (10) into account, we obtain an expression for the elastic constants in (13) in terms of the force constants of the lattice:

$$\begin{aligned} c_0^{\nu\alpha\mu\beta} &= -\frac{1}{2V_A} S_{0\chi\sigma\rho\tau}^{\nu\alpha\mu\beta} \sum_n \Phi^{\chi\sigma}(n) n^\rho n^\tau, \\ c_p^{\nu\alpha\mu\beta\lambda_1 \dots \lambda_p} &= \frac{(-1)^{p+1}}{4V_A (p+2)!} \left\{ S_{1\chi\sigma\rho\tau}^{\nu\alpha\mu\beta} \sum_n \Phi^{\lambda_p\chi}(n) n^\sigma n^\rho n^\tau n^{\lambda_1} \dots n^{\lambda_{p-1}} \right. \\ &\quad + S_{2\chi\sigma\rho\tau}^{\nu\alpha\mu\beta} \sum_n \Phi^{\chi\lambda_p}(n) n^\sigma n^\rho n^\tau n^{\lambda_1} \dots n^{\lambda_{p-1}} \\ &\quad \left. + S_{3\chi\sigma\rho\tau}^{\nu\alpha\mu\beta} \sum_n \Phi^{\chi\sigma}(n) n^\rho n^\tau n^{\lambda_1} \dots n^{\lambda_p} \right\}. \end{aligned} \quad (14)$$

In the zero long-wavelength approximation, $c_0^{\nu\alpha\mu\beta}$ is the ordinary tensor of elastic moduli.

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Note: Figure translations are in progress. See original paper for figures.

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