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DISTINGUISHING FEATURES OF ONE MODEL OF AN ELASTIC SOLID ASSOCIATED WITH THE LONG-RANGE INTERACTION AT THE MOLECULAR LEVEL

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A model of an elastic solid in the form of a system of elastically connected rigid elements is proposed. It is shown that the long-range interaction should be taken into account. The mathematical model proposed is, in essence, the physical model of a solid, which substantially broadens the range of its application.

Introduction. In [1], the author considered the mathematical model of a thin plate in the form of a system of elastically connected rigid elements. In the present paper, the physical nature of the long-range interaction of the model elements is studied. It is shown that the model can be constructed for any solid (not only for a plate). An example of the application of the model to problems of linear and nonlinear elasticity is given.

1. Some Remarks on the Interaction at the Microscopic Level. Leibfrid [2] considered comprehensively the mechanical interaction between molecules in a crystal. We point out some statements that are of interest for the present study

The character of the interaction between two atoms in a crystal lattice is illustrated in Fig. 1, which shows the potential energy φ versus the interatomic distance x (a is the lattice constant and M is the inflection point). According to [2], in calculating the macroscopic parameters (eigenfrequencies and elastic constants), it is necessary to take into account the interaction of the given atom not only with its nearest "neighbors," but also with remote "neighbors." We note that the long-range interaction is typical of many metals and dielectrics. For small deviations from the state of equilibrium, the forces can be assumed to be proportional to the displacements of the atoms. This implies that at the molecular level, the interaction can be modeled by elastic springs. In this case, the stiffness of the springs is given by $C = dF/dx$, where F is the magnitude of the force ($F_x = -d\varphi/dx$). Beyond the inflection point M, the stiffness becomes negative and decreases rapidly as x increases. According to [2, p. 131], for certain metals with a simple lattice, the stiffness of a spring that connects the atom to the second "neighbor" is tenfold smaller than the stiffness of a spring that connects it to the first "neighbor"; the ratio of the stiffnesses of the third and first "neighbors" is equal to 0.08.

We consider the model of a solid in the form of a system of elastically connected rigid elements. We show that, in accordance with the character of the interaction at the molecular level, the elastic bonds (springs) must connect each element not only to its nearest "neighbors," but also to remote "neighbors." This is the fundamental distinguishing feature of the model.

Let us consider a small solid body B1 of a definite shape, say, a parallelepiped. The dimensions of the body are chosen so that it can be considered as a set of interacting molecules. In this case, both the classical approach (for analysis of ultrasonic oscillations) and the quantum-mechanical approach (for analysis of thermal process) are applicable. We assume that the body is the single crystal of a cubic system with a simple elementary lattice (in our opinion, this restriction does not affect the final results).

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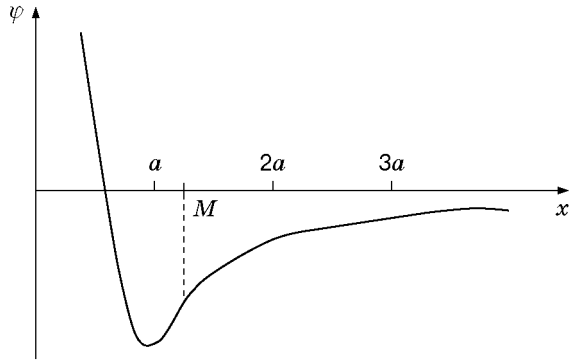

Fig. 1

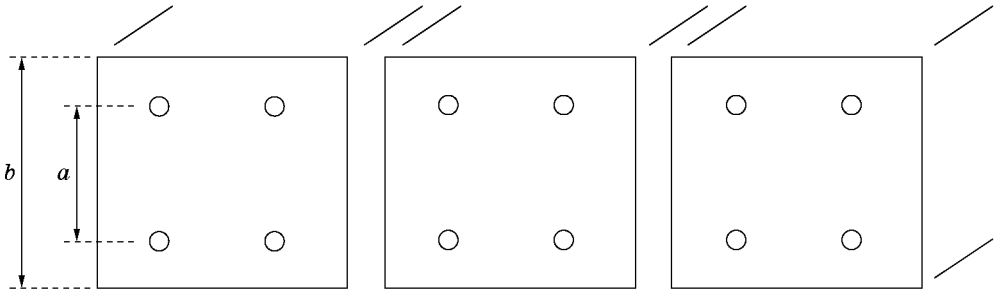

Fig. 2

We construct the physical model M1 of the body B1. The construction involves the following three stages.

1. We construct a cube (Fig. 2) for each group of eight atoms (elementary cell). Each atom in the cube is connected to all the atoms of the neighboring cubes and to those of the cubes adjacent to the neighboring cubes by means of springs modeling the interatomic interaction. The atoms are fixed in each cube. The number of cubes is denoted by N.

2. The atomic mass is uniformly distributed in the cube. The ends of the springs are fixed, and the substance of the cube imposes no restrictions on the deformation of the springs. The dimensions of the cube are chosen in such a way that its central moments of inertia are equal to the sum of the moments of inertia of the molecules. This implies that the cube edge is given by $b = a\sqrt{3}$ [a is the intermolecular distance (the lattice constant)].

3. Since the substance of the cube is assumed to be immovable relative to the cube, we can assume that the attachment points of the springs are displaced at the cube surface along the line of strings, whereas the orientation and stiffnesses of the springs remain the same. If the line of the spring moving to the "neighbor of the neighbor" intersects the space of the latter, we assume that this space imposes no restrictions on the deformation of the spring. In the case of relatively large displacements of the cubes (static problem), the attachment points of the springs are displaced.

The model M1 is approximate, since the displacements of eight molecules are determined by the displacement of the cube, i.e., the number of degrees of freedom is decreased. We show that the lower frequencies of the model M1 are close to those of the body B1 with sufficient accuracy. (By sufficient accuracy we mean the real accuracy of calculations in the theory of elasticity, which does not exceed the accuracy at which the elastic constants are determined experimentally.)

In the general case, the proof of this statement is laborious; therefore, we focus our attention on examples and qualitative reasoning. It is known that the lower frequencies of a system of elastically connected rigid units are determined mainly by the stiffness of the most pliable springs. Even though the stiffnesses of the springs differ by tenfold or more, the springs of large stiffness have little effect on the lower frequencies

and, therefore, they can be replaced by rigid connections. We consider an example. A linear chain consists of 12 point masses of 0.1 kg each. The masses are connected to an immovable base and to one another by means of 12 springs with alternating stiffnesses of 100 N/m and 1000 N/m (beginning with the spring of stiffness 100 N/m). The eigenfrequencies are as follows: 0.824, 2.435, 3.925, 5.227, 6.242, 6.893, 22.53, 22.66, 22.89, 23.15, 23.39, and 23.55 Hz. Replacing the springs of stiffness 1000 N/m by rigid connections, we obtain a system with six degrees of freedom whose eigenfrequencies are 0.858, 2.524, 4.043, 5.328, 6.303, and 6.911 Hz. The first frequencies of the two systems differ by about 4%. Obviously, as the number of degrees of freedom of the initial system B1 increases (and, hence, N increases), the initial part of the spectrum of the model M1 is extended, which can be assumed to coincide with the initial part of the spectrum of the body B1, and the accuracy of calculations is improved.

We now consider the body B2, which is geometrically similar to the body B1 and whose dimensions exceed the B1 dimensions considerably (by a factor of λ). Its material can be assumed to be continuous (the microstructure is not taken into account). We also assume that the B2 is a single crystal without defects and inclusions, as is B1.

We construct the physical model M2 of the body B2. The B2 is modeled by a system of N rigid cubes connected to one another by springs as in M1. The set of springs is the same as in M1, but their stiffnesses are not known in advance. The density of the M1 and M2 material is the same, and their dimensions differ by a factor of λ.

We show that the model M2 can be used to calculate the mechanical characteristics of the body B2.

1. The eigenfrequency spectra (at least, their low-frequency regions) of B1 and B2 are similar. Indeed, the eigenfrequencies are determined by the number of wavelengths or their parts placed on a certain characteristic dimension. For example, for free vibrations of a parallelepiped, three lower eigenfrequencies are equal to the ratio of the velocity of sound to the wavelengths (to the doubled lengths of the parallelepiped edges). Since the velocities of sound in B1 and B2 are the same and the corresponding wavelengths are proportional to the dimensions of the bodies, the ratio τ of the corresponding oscillation periods of the bodies B1 and B2 is proportional to the ratio of the linear dimensions, i.e., $\tau = \lambda$.

2. As was noted above, the lower eigenfrequencies of the body B1 and those of the model M1 coincide.

3. By construction, the models M1 and M2 are geometrically similar and the ratio of the linear dimensions of the models M1 and M2 is equal to λ. We require that the models be completely similar physically, i.e., we require that the corresponding masses and times satisfy a certain relation. The stiffnesses of the M2 springs are undetermined (the grid of the M2 springs is similar to that of the M1 springs). For similarity, the stiffness ratio is expressed with the use of the dimensional formula for stiffness $[C] = [M]/[T^2]$. Hence, we have $\mathrm{C2/C1} = (m_2/m_1)/(t_2/t_1)^2 = \lambda^3/(\tau')^2$. Choosing the stiffnesses such that their ratio is equal to λ, we obtain $\tau' = \lambda$.

4. It follows from the aforesaid that $\omega_i(\mathrm{T2})/\omega_i(\mathrm{T1}) = \omega_i(\mathrm{M2})/\omega_i(\mathrm{T1})$ ($i = 1, 2, \ldots, i \ll N$), whence $\omega_i(\mathrm{T2}) = \omega_i(\mathrm{M2})$. Consequently, the low-frequency parts of the spectra of the body B2 and the model M2 coincide. Thus, the model M2 can serve as a model of B2.

As for the equality $\omega_i(\mathrm{T2}) = \omega_i(\mathrm{M2})$, we consider it as an approximate equality. The error is due to the replacement of the stiffest springs in the B1 by absolutely rigid connections in the M1, which implies that $\omega(\mathrm{M1}) > \omega(\mathrm{T1})$. As the temperature increases (from absolute zero), the inequality becomes weaker inasmuch as the role played by stiff springs in mechanical processes is reduced.

Since the models M1 and M2 are similar, in the model M2, as in M1, the long-range interaction is modeled, i.e., each element is elastically connected not only to its nearest "neighbors," but also to the "neighbors of the neighbors." This statement is fundamental: the neglect of the long-range interaction is, apparently, responsible for the fact that models of this type have not been further developed.

2. The Model of a Thin Plate (Small Deflections). The author [1] developed the model of a thin plate in the form of a system of N elastically connected rigid square elements. We list the main parameters and characteristics of the model.

1. The plate plane is horizontal. Four horizontal-action springs with stiffness S1 are attached to each side of the element (two springs are attached to the upper part of the side and the other two are attached to the lower part to model the bending moment). Moreover, two vertical-action springs with stiffness C1 are attached to each side of the element. These springs connect the adjoining sides of the neighboring elements. At each angular point of the element, one vertical-action spring with stiffness C2 and four horizontal-action springs with stiffness S2 are attached [two of the latter springs act in the direction of one side of the element, whereas the other two act in the direction of the other (adjoining) side]. Springs of the types C2 and S2 connect the corners of the given element to the corners of the adjoining element. And, finally, the springs with stiffnesses S3, S4, and S5 are attached to each side of the element and are arranged in two layers, each of which contains five springs. They connect the side of the given element to the parallel sides of five remote elements. The springs are shown schematically in [1].

2. Each element has three degrees of freedom: the vertical displacement and rotations about two horizontal axes. The frequency equations for the system of elements have the form

$$\sum_{k=1}^{3N} B_{ik}q_k = \omega^2 \sum_{k=1}^{3N} A_{ik}q_k \qquad (i = 1, 2, \ldots, 3N), \tag{1}$$

where B is the potential-energy matrix, A is the kinetic-energy matrix, and q are the generalized coordinates. For a continuous plate, we have the equation for the deflection W

$$\Delta\Delta W = \rho\omega^2 hW/D, \tag{2}$$

in which ρ is the density, h is the thickness, $D = Eh^3/[12(1-\nu^2)]$, and $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$.

The stiffnesses of the springs are unknown. They can be found if we require that Eqs. (1) coincide with Eqs. (2) in the limit (as $N \to \infty$) (for details, the reader is referred to [1]).

3. For a square element, the stiffnesses of the springs are as follows: S1 $= 1.283\,33KD$, S2 $= -0.083\,33KD$, S3 $= 0.108\,33KD$, S4 $= -0.166\,66KD$, S5 $= 0.093\,75KD$, C1 $= (4/d^2)D$, and C2 $= (2/d^2)D$, where $K = 2/h^2$ and d is the side of the element. These values are used to construct the potential-energy matrix B. Solving system (1), we obtain the eigenfrequencies and eigenmodes of vibrations. It is noteworthy that the stiffnesses of two springs that model the long-range action have negative values (as in the case of interatomic interaction).

An analysis of the model shows its satisfactory accuracy; at least, the accuracy in determining the lower frequencies is higher than that of the COSMOS M program (in both cases, a clamped plate with a 12×12 partition was considered). In determining the tenth and first frequencies, the errors are about 10% and smaller than 0.1%, respectively.

3. The Model of a Thin Plate (Large Deflections). By construction, the model M2 can be considered as a physical model. However, the physical model of a thin plate must be applicable to both large and small deflections. The case of small deflections is considered in Sec. 2, where Eqs. (2) were used only to determine the stiffness of the model springs [by comparison with Eqs. (1)]. We now show that the model is applicable to analysis of large deflections in static problems. The following preliminary remarks should be made.

1. For small deflections, each element has three degrees of freedom. For large deflections, each element has six degrees of freedom (two horizontal displacements and rotations in the horizontal plane are also taken into account).

2. In the case of small deflections, the springs of the model can be divided into two groups, namely, horizontal- and vertical-action springs. However, when the elements rotate, the springs rotate as well; therefore, to model large deflections, one should replace the rotating springs by an equivalent system of vertical and horizontal springs so that the stiffness of the springs will depend on rotations of the elements.

3. In the case of large deflections, the distances between the elements change in such a manner that the horizontal (upper and lower) springs undergo elongations of the same sign.

Thus, an equation that describes large deflections of the model must differ from that describing small deflections. We derive this equation. We recall that the small static deflections are found from the equation

$$\sum_{i=1}^{3N} B_{ik}q_i = Q_k \qquad (k = 1, 2, \ldots, 3N), \tag{3}$$

where Q are the generalized external forces.

We assume that the expression for the potential energy of the system of elements has a uniform quadratic form:

$$\Pi = \frac{1}{2}\sum_{i=1}^{6N}\sum_{k=1}^{6N} B_{ik}q_iq_k,$$

where the components of the matrix B depend on the coordinates.

We use the principle of virtual displacements:

$$-\delta\Pi + \sum_{m=1}^{6N} Q_m\delta q_m = 0. \tag{4}$$

Substituting the potential-energy variation

$$\delta\Pi = \frac{1}{2}\sum_{i=1}^{6N}\sum_{k=1}^{6N}\delta(B_{ik}q_iq_k) = \frac{1}{2}\sum_{i=1}^{6N}\sum_{k=1}^{6N}(\delta B_{ik})q_iq_k + \sum_{i=1}^{6N}\sum_{k=1}^{6N} B_{ik}q_i\delta q_k$$

into (4), we obtain

$$\sum_{i=1}^{6N}\sum_{k=1}^{6N} B_{ik}q_i\delta q_k + \frac{1}{2}\sum_{i=1}^{6N}\sum_{m=1}^{6N}[(\delta B_{im})q_iq_m] = \sum_{k=1}^{6N} Q_k\delta q_k. \tag{5}$$

Substitution of $\delta B_{im} = \sum\limits_{k=1}^{6N}\dfrac{\partial B_{im}}{\partial q_k}\,\delta q_k$ into (5) gives

$$\sum_{k=1}^{6N}\left[\sum_{i=1}^{6N} B_{ik}q_i - Q_k + \frac{1}{2}\sum_{i=1}^{6N}\sum_{m=1}^{6N}\frac{\partial B_{im}}{\partial q_k}\,q_iq_m\right]\delta q_k = 0.$$

Hence

$$\sum_{i=1}^{6N} B_{ik}q_i = Q_k + \Phi_k, \qquad \Phi_k = -\frac{1}{2}\sum_{i=1}^{6N}\sum_{m=1}^{6N}\frac{\partial B_{im}}{\partial q_k}\,q_iq_m \qquad (k = 1, 2, \ldots, 6N). \tag{6}$$

A series of numerical experiments was performed. The problem of a 120 × 120 mm clamped thin plate bent by a uniformly distributed load was considered (h is the plate thickness). The plate material was glass-cloth-base laminate with $E = 3 \cdot 10^{10}$ Pa and $\nu = 0.28$. Equations (6) were solved iteratively. A 12 × 12 partition of the plate was used. Table 1 lists calculation results for deflection of the plate center [$\sigma_0 = 2.5 \cdot 10^4$ Pa, W_0 is the value calculated by formulas (3) (small deflections and $B_{ik} = \text{const}$), W is the value calculated by formulas (6) (large deflections), W_{theor} is the theoretical value [3], $\Delta W = W_{\text{theor}} - W$, and $\Delta = [(W_0/W)_{\text{theor}} - W_0/W]/(W_0/W)_{\text{theor}}]$. For $h = 1.5$ mm and the above value of the load σ_0, we have $(W_0)_{\text{theor}} = 0.702$ mm. The calculation results are compared with the solution of the problem W_{theor} given in [3], which, in our case, is found from the equation $5.583(W_{\text{theor}}/h)^3 + 71.840(W_{\text{theor}}/h) = (\sigma/E)(d/h)^4$. For comparison, the values of the deflection W_0 predicted by the linear theory are also given. It should be noted that, for $W/W_0 > 1.9$, the iterative process [solution of Eq. (6)] diverges. This can be attributed to the fact that the physical model becomes unstable; as applied to the prototype, this can imply the onset of plastic deformation.

TABLE 1

h, mm	σ/σ_0	W_0, mm	W, mm	W_{theor}	$\Delta W/W_{\text{theor}}$, %	W_0/W	$(W_0/W)_{\text{theor}}$	Δ, %
6	64	0.690	0.686	0.702	2.28	1.006	1.008	0.20
	320	3.450	3.071	3.138	2.13	1.123	1.128	0.44
	640	6.901	5.127	5.196	1.33	1.346	1.362	1,38
	960	10.350	6.542	6.642	1.50	1.582	1.599	1.06
	1408	15.180	8.092	8.166	0.91	1.875	1.907	1.70
3	8	0.690	0.666	0.693	3.90	1.036	1.022	−1.37
	40	3.450	2.580	2.600	0.77	1.337	1.362	1.83
	64	5.520	3.423	3.447	0.70	1.623	1.643	1.22
	80	6.901	3.890	3.888	−0.05	1.774	1.821	2.58
	96	8.280	4.283	4.269	−0.33	1.930	1.990	3.01
1.5	1	0.690	0.616	0.651	5.37	1.120	1.087	−3.03
	5	3.450	1.950	1.940	−0.50	1.789	1.840	1.76
	6	4.140	2.150	2.135	−0.75	1.926	1.990	3.20
15	$2 \cdot 10^4$	13.80	10.617	11.175	5.00	1.302	1.267	2.68

Conclusions. A model of an elastic solid in the form of a system of rigid elastically connected elements has been developed. The main distinguishing feature of the model is that it is essentially a physical model and, therefore, it is applicable to a wide range of problems. For example, the plate model in the form of a system of elastically connected rectangular elements can be used to study the static and dynamic problems of plates under small and large displacements and plane stresses. The physical model is governed by a system of algebraic equations (mathematical model). The use of this model can be advantageous in solving a number of complex problems (for example, in analysis of thick plates and shells).

The elastic connections in the model considered can be determined by analyzing the forces of interatomic interaction, but this problem of applied physics has not yet been solved in a form acceptable for practice. However, these connections can be determined by applying the model to the simplest cases and comparing equations of types (1) and (2), as in the case of a thin plate.

The distinguishing feature of the model is modeling of the long-range interaction, for which there are physical (see Sec. 1) and formal reasons: ignoring the long-range interaction does not allow one to obtain a reasonably accurate solution, i.e., Eqs. (1) and (2) do not coincide in the limiting case. It is noteworthy that in the degenerate cases (flexible thread or membrane), the long-range interaction does not occur.

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