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MECHANICS

Continual Model of Deformation of Graphene

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Abstract—A single-layer graphene sheet is studied. It is assumed that the total potential energy of the system under consideration consists of four parts. First, the energy of stretching of the bond between two neighboring atoms (the Morse potential). Second, the energy of variations in the angle between three neighboring atoms (the Brenner potential). Third, the energy needed to remove an atom from the plane defined by three neighboring atoms. Fourth, the energy of the torsion of four neighboring atoms. The van der Waals forces are neglected. Only small strains are considered. In the long-wavelength approximation, the two-dimensional extension and flexion energy is derived. As a result, an equivalent plate with corresponding extension and flexion moduli is obtained. The free vibration frequencies of a rectangular plate are found. The stability under the compression in the plane of the plate is studied. To that end, the tangential stresses are complemented with nonlinear terms depending on the transverse displacements. The results of this work are compared with the results of other authors obtained by the methods of molecular dynamics.

Keywords: graphene, stiffness, vibrations, stability.

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1. INTRODUCTION

During the last decade, graphene has been actively used in nanotechnology. Single-layer graphene sheet is an object on which the methods of studying the deformation, dynamics, and strength of more complex objects of nanomechanics, including graphite, fluorographene, nanotubes, and fullerene, have been developed. The basic method is the method of particle dynamics [1], in which the motion of a large number of interacting particles is numerically simulated. Different models (potentials) of interaction are used. The model of pairwise force interaction, when the potential depends only on the distance between particles, proves to be inconsistent for graphene because it leads to an unstable equilibrium configuration [2].

To study the tangential strain of grapheme, a model of pairwise moment interaction was proposed [2–5], in which each particle has three degrees of freedom, i.e., two translational and one rotational. In addition to the force interaction, the moment of interaction depending on the particle rotation angles is introduced. Based on this model, the stability of graphene on large stains was studied [6], and the propagation of plane waves in graphene was considered [7].

An alternative is the model of three-particle interaction [8, 9], in which, in addition to the force interaction, the expression of elastic energy involves a term that depends on the variations in the angle between three particles. It should be noted that, after the averaging, the model of paired interaction leads to Koser's two-dimensional moment medium and the model of three-particle interaction leads to an isotropic two-dimensional medium [7].

For describing the flexion strain, in addition to the pairwise and three-particles interactions, the four-particle interaction is introduced [10–13], which takes into account the energy needed to remove a particle from the plane defined by three other particles. This approach is employed in the present paper.

These potentials make it possible to construct the dynamic equations of a system of particles. As a result of the numerical integration, the problems of the free vibrations and dynamic loss of stability have been solved [13]. For the problem of free vibrations of a rectangular plate, approximate formulas for the vibration frequencies constructed by the least-square approximation in the analysis of the dynamics of a system of particles are presented in [12].

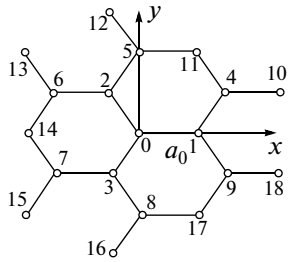

Fig. 1. Interacting points.

The aim of the present work is to construct a model of a two-dimensional continuous medium describing the deformation of a graphene sheet in the long-wavelength approximation. The potential energy is represented as a sum of four terms taking into account the variation in the distances between particles and other deformations defined by the displacement of the nearest neighbors of the given particle. The van der Waals forces and the temperature motion of particle are not taken into account. For small strains, this model describes the tangential and flexion strains, vibrations of graphene, and the stability of its plane form under tangential strains. For studying the stability, nonlinear Carman-type terms are introduced that are proportional to the squares of small rotation angles as particles exit the graphene plane. The model constructed makes it possible to speak of the existence of an equivalent plate, to which the known methods of study can be applied.

It should be added that, in [14], a two-dimensional model of nonlocal interaction was proposed, in which the discrete structure of the medium was simulated by the action of the operator $L = 1 - a^2\Delta$ on ordinary stresses, where Δ is the Laplace operator and a is a small factor. This model is not discussed here in detail.

2. MODEL OF INTERACTION BETWEEN ATOMS OF GRAPHENE

Let us consider small strains and vibrations of a single-layer graphene sheet. In the equilibrium position, the particles form a plane system of regular hexagons with a side length a_0. We assume that each particle has three degrees of freedom, two of which describe the displacements in the graphene plane, while one describes the displacements from the plane. Neglecting the van der Waals forces, we can write the elastic interaction energy Π as a sum of four terms as follows [13]:

$$\Pi = \Pi_1 + \Pi_2 + \Pi_3 + \Pi_4. \tag{2.1}$$

The potential Π_1 takes into account the variations in the distances between the pairs of particles (e.g., the distance *01*), the potential Π_2 takes into account the variation in the angles between the triples of particle (e.g., the angle *102* in Fig. 1), the potential Π_3 describes the energy needed to remove a particle from the plane containing three its nearest neighbors (e.g., particle *0* from the plane *123*), and the potential Π_4 describes the torsion energy of a chain of particle quadruples and depends on the variation in the angle between two planes (e.g., for the chain *0-1-4-10* on the angle between the planes *0-1-4* and *1-4-10*).

Let us consider the energy corresponding to particle *0*. Assuming the strains to be small, in the potentials Π_1, Π_2, and Π_3, we take into account the influence of only three nearest neighbors of point *0* and, in the potentials Π_4, of the chain consisting of point *0* and its nearest neighboring points (there are 12 such chains).

In the general case, the potential Π_1 is defined by a function of the distance r (Lennard–Jones potential [1], Morse potential, etc.). For small deformations, we will take

$$\Pi_1 = \frac{1}{2}c_1e^2, \tag{2.2}$$

where c_1 is the elastic constant and e is the strain of the segment that connects the particles. Similarly, for small strains, we will take the representation of the Brenner potential [9]

$$\Pi_2 = \frac{1}{2}c_2(\Delta\varphi)^2, \tag{2.3}$$

where c_2 is the elastic constant and $\Delta\varphi$ is the variation in the angle between particles (e.g., the angle *102*). The potentials Π_3 and Π_4 in the case of small strains will be taken in the form

$$\Pi_3 = \frac{1}{2}c_3\delta_3^2, \quad \Pi_4 = \frac{1}{2}c_4\delta_4^2, \tag{2.4}$$

where δ_3 and δ_4 are the distances from the point *0* to the planes passing through the points *123* and *1-4-10*, respectively.

3. THE TANGENTIAL STRAIN POTENTIAL ENERGY

Let us consider the tangential strain energy defined by the potentials Π_1 and Π_2. Take the origin of coordinates at the point *0*. Let u_i, v_i, and w_i be the projections of the displacements r_i of the points *1*, *2*, and *3* onto the axes of the Cartesian coordinate system *Oxyz* with the origin at the point *0*. The coordinates of the points after the deformation have the form

$$x_i = x_i^0 + u_i, \quad y_i = y_i^0 + v_i, \quad z_i = w_i, \quad i = 1, 2, 3, \tag{3.1}$$

where x_i^0, y_i^0 are the coordinates of the same points before the deformation, i.e.,

$$x_i^0 = \alpha_i a_0, \quad y_i^0 = \beta_i a_0, \quad \alpha_i = \cos\frac{2\pi(i-1)}{3}, \quad \beta_i = \sin\frac{2\pi(i-1)}{3}, \quad i = 1, 2, 3. \tag{3.2}$$

According to formulas (2.2) and (2.3), for the three nearest points, we obtain

$$\begin{gathered}\Pi_1 = \frac{1}{2}c_1(e_1^2 + e_2^2 + e_3^2), \quad e_i = \frac{|\Delta\mathbf{r}_i|}{a_0}, \quad \Delta\mathbf{r}_i = \mathbf{r}_i - \mathbf{r}_i^0, \quad i = 1, 2, 3,\\ \Pi_2 = \frac{1}{2}c_2((\Delta\varphi_{12})^2 + (\Delta\varphi_{23})^2 + (\Delta\varphi_{31})^2),\end{gathered} \tag{3.3}$$

where e_1, e_2, and e_3 are the strains of the segments *01*, *02*, and *03*.

The variations $\Delta\varphi_1$, $\Delta\varphi_2$, and $\Delta\varphi_3$ in the angles *102*, *203*, and *301* under the strain are found from the relation

$$\Delta\mathbf{r}_i \cdot \Delta\mathbf{r}_j = |\Delta\mathbf{r}_i||\Delta\mathbf{r}_j|\cos\left(\frac{2\pi}{3} + \Delta\varphi_{ij}\right). \tag{3.4}$$

Let us find the approximate expression of the tangential strain energy for small strains. We have

$$\begin{gathered}e_i = \frac{x_i^0 u_i + y_i^0 v_i + w_i^2/2}{a_0^2},\\ \Delta\varphi_{ij} = -\frac{2}{\sqrt{3}}\left(\frac{x_i^0 u_j + x_j^0 u_i + y_i^0 v_j + y_j^0 v_i + w_i w_j}{a_0^2} + \frac{1}{2}(e_i + e_j)\right).\end{gathered} \tag{3.5}$$

The approximate formulas for e_i and $\Delta\varphi_{ij}$ involve terms linear with respect to u_i and v_i and term of the second order of smallness with respect to w_i. The latter must be taken into account when considering the stability of a graphene sheet on a tangential strain.

Let us make *assumption 1*: there are smooth functions $u(x, y)$, $v(x, y)$, and $w(x, y)$ describing the displacements of points.

Then,

$$u_i = a_0(\alpha_i u_{,x} + \beta_i u_{,y}), \quad v_i = a_0(\alpha_i v_{,x} + \beta_i v_{,y}), \quad w_i = a_0(\alpha_i w_{,x} + \beta_i w_{,y}), \tag{3.6}$$

where $u_{,x} = \partial u/\partial x$ etc. are the partial derivatives. In this notation, we obtain the following expression of the energies Π_1 and Π_2:

$$\Pi_1 = \frac{3c_1}{16}(3u_{,x}^2 + 2u_{,x}v_{,y} + 3v_{,y}^2 + \omega^2 + u_{,x}(3w_{,x}^2 + w_{,y}^2) + v_{,y}(w_{,x}^2 + 3w_{,y}^2) + 2\omega w_{,x}w_{,y}),$$
$$\Pi_2 = \frac{9c_2}{16}(u_{,x}^2 - 2u_{,x}v_{,y} + v_{,y}^2 + \omega^2 + u_{,x}(w_{,x}^2 - w_{,y}^2) + v_{,y}(w_{,y}^2 - w_{,x}^2) + 2\omega w_{,x}w_{,y}), \tag{3.7}$$

where $\omega = u_{,y} + v_{,x}$ and small terms with the factors $w_{,x}^4$, $w_{,x}^2w_{,y}^2$, and $w_{,y}^4$ are discarded.

Let us introduce the tangential strain energy density per unit area as

$$U_{12} = \frac{1}{\Delta S}\left(\frac{1}{2}\Pi_1 + \Pi_2\right), \quad \Delta S = \frac{3\sqrt{3}a_0^2}{4}. \tag{3.8}$$

Here, ΔS is the area per one particle. The factor 1/2 was introduced because the energy Π_1 is taken into account twice.

The tangential stresses are found by the formulas

$$\sigma_{xx} = \frac{\partial U_{12}}{\partial u_{,x}} = E(u_{,x} + \nu v_{,y}) - \frac{3}{32}(\hat{c}_1(3w_{,x}^2 + w_{,y}^2) + 6\hat{c}_2(w_{,x}^2 - w_{,y}^2)),$$
$$\sigma_{yy} = \frac{\partial U_{12}}{\partial v_{,y}} = E(v_{,y} + \nu u_{,x}) - \frac{3}{32}(\hat{c}_1(3w_{,y}^2 + w_{,x}^2) + 6\hat{c}_2(w_{,y}^2 - w_{,x}^2)), \tag{3.9}$$
$$\sigma_{xy} = G\omega + \frac{3}{16}(\hat{c}_1 + 6\hat{c}_2)w_{,x}w_{,y},$$

where

$$E = \frac{9(\hat{c}_1 + \hat{c}_2)}{8}, \quad \nu = \frac{\hat{c}_1 - 6\hat{c}_2}{3(\hat{c}_1 + 2\hat{c}_2)}, \quad G = \frac{3(\hat{c}_1 + 6\hat{c}_2)}{16}, \quad \hat{c}_1 = \frac{c_1}{\Delta S}, \quad \hat{c}_2 = \frac{c_2}{\Delta S} \tag{3.10}$$

and the relation $G = E(1 - \nu)/2$ holds. Therefore, if $w \equiv 0$, we obtain a two-dimensional isotropic continuous medium.

4. POTENTIAL ENERGY OF THE FLEXION STRAIN

Let us find the strain energy at the point *0*. We will consider the long-wavelength approximation and assume that, in the vicinity of the point *0*, the neighboring points are situates on the second-order surface

$$z = f(x, y) = \frac{1}{2}k_1x^2 + \tau xy + \frac{1}{2}k_2y^2, \tag{4.1}$$

where k_1, k_2, and τ are the curvatures and the torsion of surface (4.1). Calculating the distances $z_0 = \delta_3$ and $z_0 = \delta_4$ entering into formulas (2.4), we find the sought energy $\Pi_{34} = \Pi_3 + \Pi_4$. In this case, the energy Π_4 consists of 12 terms. The chains *0-1-4-11*, *0-1-4-10*, *0-1-9-18*, and *0-1-9-17*, which form four terms and contain the segment *01* are shown in Fig. 1. In a similar manner, eight chains contain the segments *02* and *03*. Altogether, the interaction of particle *0* with 18 particles is taken into account (Fig. 1). The distances z_0 are found from the condition obtained by equating to zero the third-order determinant

$$\begin{vmatrix} x_i & y_i & z_i - z_0 \\ x_j & y_j & z_j - z_0 \\ x_k & y_k & z_k - z_0 \end{vmatrix} = 0, \tag{4.2}$$

where i, j, and k are the numbers of points on the plane the distance to which is calculated.

The sum of the 13 above-mentioned terms yields the energy per one point:

$$\Pi(k_1, k_2, \tau) = \frac{c_3a_0^2}{32}(k_1 + k_2)^2 + \frac{3c_4a_0^2}{2}(7k_1^2 - 2k_1k_2 + 7k_2^2 + 16\tau^2). \tag{4.3}$$

As above, the flexion strain potential energy density U_{34} is expressed by formula (4.3) in which c_3 and c_4 are replaced by

$$\hat{c}_3 = \frac{c_3}{\Delta S}, \quad \hat{c}_4 = \frac{c_4}{2\Delta S}, \quad \Delta S = \frac{3\sqrt{3}a_0^2}{4}. \tag{4.4}$$

In this case, it is taken into account that chain's energy enters into the expression twice as the two ends of the chain are considered.

5. TOTAL POTENTIAL ENERGY

The total potential energy U of the system can be found by the summation of the tangential and flexion potential energies over all particles. Assuming that the energy density varies little from one point to another, replace the summation by the integration over the surface S of the plate. As a result, we obtain

$$U = \iint_S (U_{12} + U_{34})dxdy. \tag{5.1}$$

After some transformation, the energy can be written in the form

$$U = \frac{E}{2}\iint_S \left(u_{,x}^2 + 2\nu u_{,x}v_{,y} + v_{,y}^2 + \frac{1-\nu}{2}(u_{,y} + v_{,x})^2\right)dxdy$$

$$+ \frac{D}{2}\iint_S (w_{,xx}^2 + 2\nu_b w_{,xx}w_{,yy} + w_{,yy}^2 + 2(1-\nu_b)w_{,xy}^2)dxdy \tag{5.2}$$

$$+ \frac{1}{2}\iint_S (\sigma_{xx}w_{,x}^2 + 2\sigma_{xy}w_{,x}w_{,y} + \sigma_{yy}w_{,y}^2)dxdy,$$

where the quantities E and ν are defined by formulas (3.10), the partial derivatives $w_{,xx}$, $w_{,yy}$, and $w_{,xy}$ equal the curvatures and torsion of surface (4.1),

$$D = \frac{a_0^2(\hat{c}_3 + 168\hat{c}_4)}{16}, \quad \nu_b = \frac{\hat{c}_3 - 24\hat{c}_4}{\hat{c}_3 + 168\hat{c}_4}, \tag{5.3}$$

and the tangential stresses σ_{xx}, σ_{yy}, and σ_{xy} are calculated by formulas (3.9), in which we set $w = 0$.

Potential energy (5.2) corresponds to a plate subjected to tangential and flexion strains, E is the extension stiffness, and D is the bending stiffness. The Poisson coefficients ν and ν_b proved to be different on the tangential strain and flexion. Using the known formulas for a plate

$$E = \frac{E_0 h_0}{1-\nu_0^2}, \quad D = \frac{E_0 h_0^3}{12(1-\nu_0^2)}, \tag{5.4}$$

we can introduce the effective thickness h_0 of a graphene sheet by the formula

$$h_0 = \frac{\sqrt{12D}}{E}. \tag{5.5}$$

According to the Hamilton–Ostrogradski principle, varying the functional

$$\delta\int_{t_1}^{t_2}(T-U)dt = 0 \tag{5.6}$$

with respect to u, v, and w yields the equations of motion and the boundary conditions. Here, T is the kinetic energy of the system

$$T = \frac{\rho}{2}\iint_S (u_{,t}^2 + v_{,t}^2 + w_{,t}^2)dxdy, \quad \rho = \frac{m_0}{\Delta S}, \tag{5.7}$$

where ρ is the particle density per unit area and m_0 is the particle mass.

In a number of cases, the continual approach proposed here makes it possible to obtain the explicit solution. The main errors of this approach come from assumption 1 that there are smooth functions $u(x, y)$, $v(x, y)$, and $w(x, y)$ that describe the displacement of points in the vicinity of the given point and from the neglect of the interaction with remote points. In accordance with the long-wavelength approximation employed in this work, the error increases with a reduction in the strain wavelength. Another source of errors is that the expression of energy Π_4 (3.3) can only be used for particles found at a distance from the edge of at least $(2 + \sqrt{3}/2)a_0$ (Fig. 1).

The proposed continual approach is insensitive to the chirality of graphene.

6. FREE VIBRATIONS OF A RECTANGULAR GRAPHENE SHEET

Let us consider a rectangular graphene sheet with the dimensions $0 \le x \le a$, $0 \le y \le b$. In order to study the transverse displacements, we will find the variations in functional (5.6) with respect to w. Integrating by parts, we obtain

$$\begin{aligned} &\int_0^a\int_0^b (D\Delta\Delta w + \rho w_{,tt} - F)\delta w dxdy \\ &+ \int_0^b M_{xx}\delta w_{,x}\Big|_{x=0}^{x=a} dy + \int_0^a M_{yy}\delta w_{,y}\Big|_{y=0}^{y=b} dx \\ &- \int_0^b Q_x\delta w\Big|_{x=0}^{x=a} - \int_0^a Q_y\delta w\Big|_{y=0}^{y=b} dx + 2M_{xy}\delta w\Big|_{x=0}^{x=a}\Big|_{y=0}^{y=b} = 0, \end{aligned} \tag{6.1}$$

where

$$\begin{gathered} \Delta w = w_{,xx} + w_{,yy}, \quad F = (\sigma_{xx}w_{,x})_{,x} + (\sigma_{xy}w_{,x})_{,y} + (\sigma_{xy}w_{,y})_{,x} + (\sigma_{yy}w_{,y})_{,y}, \\ M_{xx} = D(w_{,xx} + \nu_b w_{,yy}), \quad M_{yy} = D(w_{,yy} + \nu_b w_{,xx}), \quad M_{xy} = D(1-\nu_b)w_{,xy}, \\ Q_x = D(w_{,xxx} + (2-\nu_b)w_{,xyy}) - \sigma_{xx}w_{,x} - \sigma_{xy}w_{,y}, \\ Q_y = D(w_{,yyy} + (2-\nu_b)w_{,xxy}) - \sigma_{xy}w_{,x} - \sigma_{yy}w_{,y}. \end{gathered} \tag{6.2}$$

Now let us consider free transverse vibrations under the assumption that the initial stresses are absent ($F = 0$) and all edges are simply supported as follows:

$$w = w_{,xx} = 0 \ \ (x = 0, x = a), \quad w = w_{,yy} = 0 \ \ (y = 0, y = b). \tag{6.3}$$

The modes of the vibrations

$$w_{mn}(x, y) = w_0 \sin\frac{m\pi x}{a_x}\sin\frac{n\pi y}{a_y}, \quad m, n = 1, 2, \ldots \tag{6.4}$$

satisfy the equation $D\Delta\Delta w + \rho w_{,tt} = 0$ and boundary conditions (6.3). They correspond to the free vibration frequencies

$$\omega_{mn} = \sqrt{\frac{D}{\rho}}\left(\frac{m^2\pi^2}{a^2} + \frac{n^2\pi^2}{b^2}\right). \tag{6.5}$$

The range of applicability of formula (6.5) is limited by the condition that the half-wavelengths a/m and a/n must be substantially greater than the minimum distance between particles:

$$\min\{a/m, b/n\} \gg a_0. \tag{6.6}$$

Otherwise, the long-wavelength approximation employed here is not applicable.

7. STABILITY OF A RECTANGULAR GRAPHENE SHEET UNDER COMPRESSION

Let us consider the static loss of stability under a uniaxial compression in the direction of the x axis [16] by setting

$$\sigma_{xx} = -p, \quad p > 0, \quad \sigma_{xy} = \sigma_{yy} = 0. \tag{7.1}$$

Assuming that the edges $x = 0$ and $x = a$ are simply supported and the edges are free, the deflection when the stability is lost can be found from the solution of the boundary value problem

$$\begin{gathered} D\Delta\Delta w + pw_{,xx} = 0, \quad w = w_{,xx} = 0 \ \ (x = 0, x = a), \\ w_{,yy} + \nu_b w_{,xx} = 0, \quad D(w_{,yyy} + (2 - \nu_b)w_{,xxy}) = 0 \ \ (y = 0, y = b). \end{gathered} \tag{7.2}$$

After the separation of variables,

$$w(x, y) = W(y)\sin\frac{\pi x}{a}, \tag{7.3}$$

we arrive at a boundary value problem that has even and odd solutions with respect to the middle $y = b/2$. For the even solution,

$$W(y) = C_1\cosh(\lambda_1(y/a - b/(2a))) + C_2\cosh(\lambda_2(y/a - b/(2a))), \tag{7.4}$$

which gives a lower value of the load, the equation for determining the critical load has the form

$$\begin{vmatrix} (\lambda_1^2 - \nu_b)\cosh(\lambda_1\eta) & (\lambda_2^2 - \nu_b)\cosh(\lambda_2\eta) \\ (\lambda_1^3 - (2 - \nu_b)\lambda_1)\sinh(\lambda_1\eta) & (\lambda_2^3 - (2 - \nu_b)\lambda_2)\sinh(\lambda_2\eta) \end{vmatrix} = 0, \tag{7.5}$$

where

$$\lambda_{1,2}^2 = 1 \pm \sqrt{\hat{p}}, \quad \hat{p} = \frac{pa^2}{D\pi^2}, \quad \eta = \frac{b}{2a}. \tag{7.6}$$

8. NUMERICAL RESULTS

Let us take the following values of parameters: particle mass $m_0 = 1.9927 \times 10^{-26}$ kg, the distance between particles $a_0 = 0.142 \times 10^{-9}$ m, and the mass per unit area $\rho = 7.608 \times 10^{-7}$ kg/m^2. We also take the stiffness coefficients from [13], which, after the linearization, in our notation, yield $\hat{c}_1 = 319.8$ N/m and $\hat{c}_2 = 33.44$ N/m. Using formulas (3.10), we find $E = 220.8$ N/m and $\nu = 0.086$. Then, we have $a_0^2\hat{c}_3 = 10.61$ N/m and $a_0^2\hat{c}_4 = 8.86$ N/m and, using formula (5.3), we obtain $D = 93.7\ a_0^2$ Nm and $\nu_b = -0.135$.

Let us consider the free vibrations of a simply supported rectangular plate with the side lengths $a = 3.266 \times 10^{-9}$ m and $b = 3.433 \times 10^{-9}$ m. Using formula (6.5), we find the first transverse vibration frequency $\nu_{11} = \omega_{11}/(2\pi) = 0.442 \times 10^{12}$ (Hz). In [13], the corresponding value obtained by the method of particle dynamics for the same plate was $\nu_{11} = 0.259 \times 10^{12}$ (Hz).

Now let us turn to the problem of stability. For the values of parameters adopted above, we find the solution of Eq. (7.5): $\hat{p} = 0.984$. Then, due to formulas (7.1) and (7.6), $\sigma_{xx} = -1.720$ (N/m), the strain $u_{,x} = \sigma_{xx}/E = -0.00779$ and the critical distance between the edges is $\Delta x = a|u_{,x}| = 2.54 \times 10^{-11}$ (m). The same problem was solved in [13] by the method of particle dynamics. The approach of two opposite sides with a given velocity was specified. At the velocity $v = 50$ (m/s), the transverse motion began at $\Delta x = 1.05 \times 10^{-10}$ (m) and, at the velocity $v = 5$ (m/s), it began at $\Delta x = 3.125 \times 10^{-11}$, i.e., the quantitative difference between our results and the results of [13] decreases with a decrease in the velocity with which the side approach one another.

9. DISCUSSION

The comparison of our results with the results of [13] says that the continual model proposed in this work leads to a stiffer plate than that given by the model based on the particle dynamics [13], because assumption 1 imposed certain constraints on the particle displacements. Let us discuss this question in more detail.

In [7], when calculating the tangential strain energy Π_{12}, of four particles *0*, *1*, *2*, and *3*, the projections u_0 and v_0 of the displacement of particle *0* were determined from the minimum energy condition (in Section 3, we adopted $u_0 = v_0 = 0$). As a result, for the elastic moduli, in contrast to (3.10), we obtain

$$\tilde{E} = \frac{3\hat{c}_1(\hat{c}_1^2 + 18\hat{c}_1\hat{c}_2 + 27\hat{c}_2^2)}{8(\hat{c}_1 + 3\hat{c}_2)^2}, \quad \hat{\nu} = \frac{\hat{c}_1^2 - 6\hat{c}_1\hat{c}_2 - 9\hat{c}_2^2}{\hat{c}_1^2 + 18\hat{c}_1\hat{c}_2 + 27\hat{c}_2^2}, \quad \tilde{G} = \frac{9\hat{c}_1\hat{c}_2(2\hat{c}_1 + 3\hat{c}_2)}{4(\hat{c}_1 + 3\hat{c}_2)^2}. \tag{9.1}$$

Releasing from the nonexisting bonds $u_0 = v_0 = 0$ reduces the tangential stiffness of the plate insignificantly. For the above-adopted values of the coefficient $\hat{c}_1$ and $\hat{c}_2$, we have

$$E/\tilde{E} = 220.8/217.2, \quad \nu/\tilde{\nu} = 0.086/0.103, \quad G/\tilde{G} = 118.8/97.6. \tag{9.2}$$

It should be noted that the Poisson coefficients ν and $\tilde{\nu}$ noticeably differ from the values 0.17–0.21 presented in [5]. The results can only be made closer by changing the coefficients c_1 and c_2 in formulas (2.2) and (2.3). For flexion strains, assumption 1 leads to an even greater error. For estimating it, let us reject the assumption that the particles lie on surface (4.1), i.e., $z_i = f(x_i, y_i)$, $i = 0, 1, \ldots, 18$. We will seek the values z_i, $(i > 0)$ for which the flexion strain energy $\Pi_{34}(k_1, k_2, \tau)$ is minimal. In this case, we will impose a restriction that the mean-square approximation of the set of points x_i, y_i, z_i by a second-order surface

$$z = f(x, y) = \frac{1}{2}k_1x^2 + \tau xy + \frac{1}{2}k_2y^2 + ax + by + c, \tag{9.3}$$

leads to the same values of k_1, k_2, and τ as obtained above. This restriction will be satisfied if we take

$$z_i = f(x_i, y_i) + \Delta z_i, \quad i = 1, 2, \ldots, 18, \tag{9.4}$$

where the increments Δz_i satisfy the three linear equations

$$\langle a_i^{(k)}\Delta z_i\rangle = 0, \quad k = 1, 2, 3, \quad \langle g_i\rangle \equiv \sum_{i=0}^{18} g_i, \tag{9.5}$$

where

$$a_i^{(1)} = x_i^2 - \frac{\langle x_i^2\rangle}{19} - x_i\frac{\langle x_i^3\rangle}{\langle x_i^2\rangle}, \quad a_i^{(2)} = x_iy_i - y_i\frac{\langle x_iy_i^2\rangle}{\langle y_i^2\rangle}, \quad a_i^{(3)} = y_i^2 - \frac{\langle y_i^2\rangle}{19} + x_i\frac{\langle x_iy_i^2\rangle}{\langle x_i^2\rangle}.$$

The approximate minimum of the flexion strain was calculated by the Monte Carlo method, when the values of Δz_i were randomly chosen. For each set of parameters k_1, k_2, and τ, 2×10^7 variants have been considered. As a result of the trial of the values of Δz_i, a significant (by 20–36%, depending on k_1, k_2, τ) reduction in the energy of interaction of particle *0* with other 18 particles from the energy Π_{34} in the case when all particles lie on surface (4.1) was noticed. This result can be improved if we take into account that the found arrangement of points close to optimal for particle *0* can be nonoptimal for other particles. Therefore, we have calculated the bending energy of the interaction of all 19 particles (Fig. 1). There were terms terms of the type of Π_3 in (2.4) and 48 terms of the type of Π_4. Depending on the parameters k_1, k_2, and τ, the results obtained by the Monte Carlo method exhibited a 5–18% reduction in the energy.

The continual model can be improved due to the choice of the stiffness parameters of the plate. At the same time, our calculations have shown that, on a flexion strain, particles are not situated on a smooth surface. In connection with this, it may be promising to use model [14], which takes into account the nonlocal interactions.

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