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Bending Stiffness of a Graphene Sheet

I. E. Berinskii[1, 2]*, A. M. Krivtsov[1, 2], and A. M. Kudarova[3]

[1] *Institute of Problems of Mechanical Engineering, RAS, St. Petersburg, 199178 Russia*
[2] *St. Petersburg State Polytechnical University, St. Petersburg, 195251 Russia*
[3] *Delft University of Technology, Delft, 2628 CN Netherlands*
** iberinsk@gmail.com*

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Abstract—The paper proposes a discrete mechanical model of monolayer graphene. A relation between parameters of the model and elastic characteristics of its equivalent continuum is derived by comparing the energy of small strains on micro- and macroscales. The relation allows one to determine the microscale interaction parameters from experimental data and, knowing the microscale parameters, to determine the mechanical properties of graphene. The main aim of the work is to estimate the bending stiffness of a graphene sheet. The proposed discrete model provides an analytical dependence of the graphene sheet bending stiffness on the microscale interaction parameters.

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1. INTRODUCTION

Recently, much efforts have been toward research and development of nanoelectromechanical systems, in particular, for finding methods to create new-generation of nanoresonators. The available quartz resonators offer a high frequency and quality factor (up to 400 MHz and 2500, respectively); however, decreasing their thickness to nanometer sizes impairs their quality due to surface effects. Moreover, there are difficulties in manufacturing thin quartz wafers with highly parallel working surfaces with the result that resonances may occur at harmonics close to operating frequencies [1]. Therefore, attention of researchers is toward creating resonators based on carbon nanostructures, in particular graphene. Graphene is a graphite monolayer containing a single layer of atoms and is the thinnest known material. Since graphene was pioneered not long ago [2], graphene resonators are in their infancy [3, 4] and there is much to do with their design and manufacture.

The mechanical properties of graphene resonators are defined by the ability of a graphene sheet to resist both tension and bending. The bending stiffness of graphene (the resistance of an elastic shell to out-of-plane bending) is its fundamental property. In the works by Peierls [5] and Landau [6], it is shown that an infinite prefect 2D crystal loses its stability under the action of thermal fluctuations. However, the presence of bending stiffness can provide additional stabilization of graphene, thus precluding its fracture.

In the membrane theory of shells with pure bending, the bending stiffness D is the proportionality factor between the bending moment M and curvature of a plate κ:

$$M = D\kappa. \tag{1}$$

The stiffness D of the plate is expressed in terms of its Young's modulus E, Poisson's ratio ν, and thickness h [7]:

$$D = \frac{Eh^3}{12(1-\nu^2)}. \tag{2}$$

However, the thickness of monolayer graphene is impossible to uniquely determine and this does not allow direct use of formula (2). Let the parameters of graphene be Eh = 340 N/m and ν = 0.17 that are obtainable from the experimental data [8]. In the context of the most common idea [9–14], we also assume that the thickness of graphene is equal to the spacing between graphene layers in graphite and is h = 0.34 nm. Thus, we obtain D = 3.37 nN · nm. However, this value is an order of magnitude higher than the bending stiffness of monolayer graphene (Table 1) estimated by other methods without using the notion of thickness: ab initio or first-principles quantum mechanical calculations and calculation with empirical interaction potentials.

It is seen from Table 1 that the bending stiffness predicted for monolayer graphene by the latter two methods has the same order of magnitude: it varies from 0.13 to 0.26 nN · nm (0.8–1.6 eV). These data are impossible to experimentally verify in the context of classical continuum theories. However, these theories are applicable to multilayer graphene and allow experimental verification of its bending stiffness. The bending stiffness of two-layer graphene was determined via electrostatic actuation of a buckled membrane (which lost its stability due to concentrated force) and was 5.7 nN · nm [18]. The authors of [19] determined the bending stiffness of a few-layer graphene membrane by indentation into a circular hole; the experimental data fit the curve described by (2). The dependence of bending stiffness on the number of layers N for a multilayer membrane was estimated as $D = 9.8N^2$ nN · nm [20]; this value was obtained by estimation of "smoothing" of a compliant corrugated substrate on which a graphene membrane was fixed. Thus, the latter two works experimentally confirm the dependence of bending stiffness on cubed thickness for multilayer membranes. However, dependence (2) is inapplicable to monolayer membranes.

The bending stiffness of covalent bonds reflects their orientation. The interaction forces are not central: a transverse force along with a longitudinal force arises. In the general case, these interactions can be described taking into account the contribution of moment interaction, in addition to force interaction, between pair particles. The interaction potentials depend on relative positions and rotations of two interacting particles. This type of moment models provides agreement with experimental data, while operating with relatively few but physically clear parameters. The approach was applied to consider pure bending of a two-dimensional multilayer nanocrystal with a triangular lattice [21] and this gave formula

$$D = A_1(N-1)N(N+1) + A_2(3N-1). \qquad (3)$$

Here A_1 and A_2 are constant factors dependent on the lattice properties. Thus, the bending stiffness of the nanocrystal is the sum of two terms, of which one vanishes for a single layer and tends to (2) for a larger number of layers. The second term is due to allowance for moment interaction in addition to force interaction. This correction term, compared to the first term, gets smaller with increasing the nanocrystal thickness but assumes significance for nanocrystals with a small number of layers and monolayer structures.

Table 1. Bending stiffness of monolayer graphene determined by different methods

Source	D, nN · nm	Method
[15]	0.24	Ab initio
[12]	0.26	
[13]	0.23	
[14]	0.13	Empirical potential
[16]	0.13	
[17]	0.22	

The present paper proposes an approach that allows estimating the bending stiffness of a single graphene layer. The approach, like the one considered earlier [21], account for moment interaction in addition to force interaction. It is taken that carbon atoms in graphene interact with each other via forces and moments. Equations describing these interactions are presented in Sect. 2.1. A transition from micro- to macrostructure is considered in Sect. 2.2. The transition makes it possible to relate the moment and force interaction stiffnesses to the elastic characteristics of the material. Thus, the bending stiffness of a graphene sheet is a function of longitudinal, transverse, bending, and torsional stiffnesses of carbon bond. A model of carbon bond—an elastic rod—is described in Sect. 2.3. The model allows one to express the bending and torsional stiffnesses of carbon bond in terms of longitudinal and transverse stiffnesses and to relate the latter stiffnesses to experimental data. The desired bending stiffness of graphene is calculated using the derived formulae in Sect. 2.4. Discussion of the results and concluding remarks are presented in Sect. 3.

2. BENDING STIFFNESS OF A GRAPHENE SHEET

2.1. Microscale Interaction

The interactions in the graphene lattice are described using the approach proposed elsewhere [21, 22]. A carbon atom in graphene is modeled by a body-point, i.e., by a material object which occupies a zero volume in space and the position of which is considered definite if its position vector and rotation tensor are given. The interaction between body-points is characterized by force and moment vectors.

Let us use a system of two body-points to model lattice atoms. In the actual configuration, their position is specified by radius vectors $\mathbf{r}_1, \mathbf{r}_2$, and orientation by rotation vectors $\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2$. In the equilibrium position, $\mathbf{r}_2 - \mathbf{r}_1 = \mathbf{r}_0$, $\boldsymbol{\varphi}_1 = 0$, $\boldsymbol{\varphi}_2 = 0$. Let $\mathbf{f}_1, \mathbf{m}_1$ be the force and moment acting on body-point 1 from the side of body-point 2 and $\mathbf{f}_2, \mathbf{m}_2$ be the force and moment acting on body-point 2 from the side of body-point 1. For these parameters, we have

$$\mathbf{f} = \mathbf{f}_1 = -\mathbf{f}_2, \quad (4)$$

$$\mathbf{m} = \mathbf{m}_1 + 1/2(\mathbf{r}_1 - \mathbf{r}_2)\times\mathbf{f}_1 = -\mathbf{m}_2 - 1/2(\mathbf{r}_2 - \mathbf{r}_1)\times\mathbf{f}_2. \quad (5)$$

For linear elastic deformation, the internal energy can be given in the following approximation:

$$U = \mathbf{f}_0\cdot\boldsymbol{\varepsilon} + \mathbf{m}_0\cdot\boldsymbol{\kappa} + 1/2\,\boldsymbol{\varepsilon}\cdot\mathbf{A}\cdot\boldsymbol{\varepsilon} + \boldsymbol{\varepsilon}\cdot\mathbf{B}\cdot\boldsymbol{\kappa} + 1/2\,\boldsymbol{\kappa}\cdot\mathbf{C}\cdot\boldsymbol{\kappa}. \quad (6)$$

The coefficients **A**, **B**, and **C** are the stiffness tensors of bonds and the vectors $\mathbf{f}_0$ and $\mathbf{m}_0$ are the initial forces. In the linear theory, the stiffness tensors are constants, with the tensors **A** and **C** being symmetric and **B** being arbitrary. The vectors $\boldsymbol{\varepsilon}$ and $\boldsymbol{\kappa}$, which are the strain vectors, are assigned the work of force and moment vectors:

$$\mathbf{f} = \mathbf{f}_0 + \mathbf{A}\cdot\boldsymbol{\varepsilon} + \mathbf{B}\cdot\boldsymbol{\kappa}, \;\; \mathbf{m} = \mathbf{m}_0 + \boldsymbol{\varepsilon}\cdot\mathbf{B} + \mathbf{C}\cdot\boldsymbol{\kappa}. \quad (7)$$

The above relations were derived using the interaction moment **m** calculated with respect to the midpoint of the segment connecting the body-points. The stiffness tensors **B** and **C** were also calculated with respect to this point. The strain vectors, in this case, have the form:

$$\boldsymbol{\varepsilon} = \mathbf{r} - \mathbf{r}_0 + 1/2\,\mathbf{r}_0\times(\boldsymbol{\varphi}_1 + \boldsymbol{\varphi}_2), \quad \boldsymbol{\kappa} = \boldsymbol{\varphi}_2 - \boldsymbol{\varphi}_1, \;\; \mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1. \quad (8)$$

Equations (7), (8) are convenient for determination of the stiffness tensors. The interaction characteristics of the examined two-particle system were calculated with respect to the centre of the system; therefore, the system has two orthogonal symmetry planes. It can be demonstrated that the stiffness tensors, in the case, have the form:

$$\mathbf{A} = C_A\mathbf{ii} + C_D\mathbf{jj}, \;\; \mathbf{B} = 0, \;\; \mathbf{C} = C_T\mathbf{ii} + C_B(\mathbf{jj} + \mathbf{kk}), \quad (9)$$

where **i**, **j**, and **k** are the orthonormal basis vectors such that the particles lie in the plane formed by the vectors **i** and **j**, **k** is orthogonal to this plane.

However, in solving specific problems, it is often convenient to use interaction moments calculated with respect to body-points. The strain vectors thus take the form

$$\boldsymbol{\varepsilon}_1 = \mathbf{r} - \mathbf{r}_0 + \mathbf{r}_0\times\boldsymbol{\varphi}_2, \;\; \boldsymbol{\kappa}_1 = \boldsymbol{\varphi}_2 - \boldsymbol{\varphi}_1, \;\; \mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1. \quad (10)$$

The force and moment vectors, in this case, can be expressed as

$$\mathbf{f}_1 = \tilde{\mathbf{f}}_0 + \mathbf{T_A}\cdot\boldsymbol{\varepsilon}_1 + \mathbf{T_B}\cdot\boldsymbol{\kappa}_1, \quad \mathbf{m}_1 = \tilde{\mathbf{m}}_0 + \boldsymbol{\varepsilon}_1\cdot\mathbf{T_B} + \mathbf{T_C}\cdot\boldsymbol{\kappa}_1. \quad (11)$$

The initial forces $\tilde{\mathbf{f}}_0$ and $\tilde{\mathbf{m}}_0$ differ from the initial forces $\mathbf{f}_0$ and $\mathbf{m}_0$, and the stiffness tensors $\mathbf{T_A}$, $\mathbf{T_B}$, and $\mathbf{T_C}$ differ from the tensors **A**, **B**, and **C**. In what follows, we consider unstressed systems, i.e., the initial forces are taken equal to zero. It is easy to check that the following relations hold true:

$$\mathbf{T_A} = \mathbf{A}, \;\; \mathbf{T_B} = \mathbf{B} - 1/2\,\mathbf{A}\times\mathbf{r}_0, \quad \mathbf{T_C} = \mathbf{C} + 1/2(\mathbf{r}_0\times\mathbf{B} - \mathbf{B}^{\mathbf{T}}\times\mathbf{r}_0) - 1/4\,\mathbf{r}_0\times\mathbf{A}\times\mathbf{r}_0. \quad (12)$$

Let us consider a more general case of particle interaction. Let the discrete structure of material represent a set of body-points which have three rotational degrees of freedom and three translational degrees of freedom; we consider the interaction of the nearest neighbors only. For simplicity, the bonds between the particles are assumed transversely isotropic. The bond strain is described by four force constants: C_A for tension, C_D for shear, C_T for torsion, and C_B for bending. The elastic strain energy of the lattice per unit lattice cell can be represented as the sum of strain energies for the bond between a certain reference particle and its nearest neighbors:

$$W = \frac{1}{2V_0}\sum_{\alpha}\Pi_\alpha, \quad (13)$$

where Π_α is the potential interaction energy for the particle and its neighbor with an index α, V_0 is the unit cell volume. In the unit lattice cell, there can be more than one particle. For example, the graphene lattice contains two particles in its unit cell.

The potential energy Π_α can be represented as the quadratic form of strain vectors and bond stiffness tensors:

$$\Pi_\alpha = \frac{1}{2}\boldsymbol{\varepsilon}_\alpha\cdot\mathbf{A}_\alpha\cdot\boldsymbol{\varepsilon}_\alpha + \boldsymbol{\varepsilon}_\alpha\cdot\mathbf{B}_\alpha\cdot\boldsymbol{\kappa}_\alpha + 1/2\,\boldsymbol{\kappa}_\alpha\cdot\mathbf{C}_\alpha\cdot\boldsymbol{\kappa}_\alpha, \quad (14)$$

where $\mathbf{A}_\alpha, \mathbf{B}_\alpha, \mathbf{C}_\alpha$ are the stiffness tensors of the bond α which contain information on the bond strain in different directions:

$$\mathbf{A}_\alpha = C_A\mathbf{n}_\alpha\mathbf{n}_\alpha + C_D(\mathbf{E} - \mathbf{n}_\alpha\mathbf{n}_\alpha), \quad \mathbf{C}_\alpha = C_T\mathbf{n}_\alpha\mathbf{n}_\alpha + C_B(\mathbf{E} - \mathbf{n}_\alpha\mathbf{n}_\alpha), \;\; a\mathbf{n}_\alpha = \mathbf{a}_\alpha. \quad (15)$$

Here **E** is the unit tensor, the vector $\mathbf{n}_\alpha = \mathbf{a}_\alpha/a$, where a is the bond length, $\mathbf{a}_\alpha$ connects two neighbor particles. The tensor **B** is equal to zero if the lattice has two mutually perpendicular symmetry planes [16], which holds true for the graphene lattice.

The strain vectors can be represented in the form [16]:

$$\boldsymbol{\varepsilon}_\alpha = \mathbf{u}_\alpha - \mathbf{u} + 1/2\,\mathbf{a}_\alpha\times(\boldsymbol{\varphi}_\alpha + \boldsymbol{\varphi}), \;\; \boldsymbol{\kappa}_\alpha = \boldsymbol{\varphi}_\alpha - \boldsymbol{\varphi}. \quad (16)$$

Here $\mathbf{u}_\alpha, \mathbf{u}$ are the displacements of the particle with an index α and reference particle, respectively; $\boldsymbol{\varphi}_\alpha, \boldsymbol{\varphi}$ are their rotations.

Equations (14), (15) can be substituted in (13) to determine the potential energy of the particle system depending on the particle position $\mathbf{u}_\alpha, \mathbf{u}$, orientation $\boldsymbol{\varphi}_\alpha, \boldsymbol{\varphi}$, initial configuration geometry $\mathbf{a}_\alpha$, and force interaction constants C_A, C_B, C_T, C_D.

2.2. Micro-to-MacroscaleTtransition

Let us correlate the displacements and rotations of a particle with those of a continuum element: $\mathbf{u} = \mathbf{u}(\mathbf{r})$, $\boldsymbol{\varphi} =$

$\boldsymbol{\varphi}(\mathbf{r})$, where $\mathbf{r}$ is the radius vector in the initial configuration. Then, the displacements and rotations of neighbor particles can be expressed as $\mathbf{u}_\alpha = \mathbf{u}(\mathbf{r}-\mathbf{a}_\alpha)$, $\boldsymbol{\varphi}_\alpha = \boldsymbol{\varphi}\times(\mathbf{r}-\mathbf{a}_\alpha)$. Let us use the long-wave approximation [23] assuming that the wavelengths are much larger than the initial interatomic distance between the nearest neighbors a_α, which is taken to be a small parameter. Then, the displacements and rotations can be represented in the form of expansions:

$$\mathbf{u}_\alpha = \mathbf{u} + \mathbf{a}_\alpha\cdot\nabla\mathbf{u} + \eta\boldsymbol{\varsigma},\ \ \boldsymbol{\varphi}_\alpha = \boldsymbol{\varphi} + \mathbf{a}_\alpha\cdot\nabla\boldsymbol{\varphi} + \eta\boldsymbol{\psi}. \quad (17)$$

Here ∇ is the nabla operator. The parameter η is equal to unity if the unit cell contains two particles and to zero if it contains one particle. The vectors $\boldsymbol{\varsigma}, \boldsymbol{\psi}$ denote the relative displacements and rotations of particles from different sublattices of the complete lattice. Expressions (17) can be substituted in the expression for energy W (13). Then, we are to find the vectors $\boldsymbol{\varsigma}, \boldsymbol{\psi}$ from the condition that they provide displacement of one sublattice relative to the other to fit the minimum strain energy:

$$\frac{\partial W}{\partial\boldsymbol{\varsigma}} = 0,\ \ \frac{\partial W}{\partial\boldsymbol{\psi}} = 0. \quad (18)$$

Once the vectors $\boldsymbol{\varsigma}, \boldsymbol{\psi}$ are determined from condition (18), the energy density of the equivalent continuum takes the form

$$W = W(\nabla\mathbf{u}, \nabla\boldsymbol{\varphi}, \boldsymbol{\varphi}, C_A, C_D, C_T, C_B). \quad (19)$$

The energy density can also be represented in the quadratic form of fourth rank stiffness tensors and strain tensors:

$$W = 1/2\ {}^2\boldsymbol{\varepsilon}\cdot\cdot{}^4\mathbf{A}\cdot\cdot{}^2\boldsymbol{\varepsilon} + {}^2\boldsymbol{\varepsilon}\cdot\cdot{}^4\mathbf{B}\cdot\cdot{}^2\boldsymbol{\kappa} + 1/2\ {}^2\boldsymbol{\kappa}\cdot\cdot{}^4\mathbf{C}\cdot\cdot{}^2\boldsymbol{\kappa}. \quad (20)$$

The strain tensors have the form:

$${}^2\boldsymbol{\varepsilon} = \nabla\mathbf{u} + \mathbf{E}\times\boldsymbol{\varphi},\ \ {}^2\boldsymbol{\kappa} = \nabla\boldsymbol{\varphi}. \quad (21)$$

To obtain relations between the microscale force interaction constants and stiffness tensor components, we are to compare the expressions for energies (19) and (20).

Now let us apply the above method to the 2D hexagonal graphene lattice. Let us introduce an orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, where the vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ lie in the lattice plane and the vector $\mathbf{e}_3$ is perpendicular to the lattice plane. Let the axes x, y, and z be codirectional with the vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$, respectively. Then, the bond direction vectors can be expressed as

$$\mathbf{n}_1 = \mathbf{e}_1,\ \ \mathbf{n}_2 = -1/2\,\mathbf{e}_1 + \sqrt{3}/2\,\mathbf{e}_2,\ \ \mathbf{n}_3 = -1/2\,\mathbf{e}_1 - \sqrt{3}/2\,\mathbf{e}_2. \quad (22)$$

The displacements and rotations can also be expanded in terms of the basis:

$$\mathbf{u} = u^x(x, y)\mathbf{e}_1 + u^y(x, y)\mathbf{e}_2 + u^z(x, y)\mathbf{e}_3,\ \ \boldsymbol{\varphi} = \varphi^x(x, y)\mathbf{e}_1 + \varphi^y(x, y)\mathbf{e}_2 + \varphi^z(x, y)\mathbf{e}_3. \quad (23)$$

So, it is easy to compare energies (19) and (20); energy (19) was obtained for the graphene lattice with regard to (22). For this purpose, we equate the factors preceding the derivatives of the displacement and rotation vector components and also those preceding the rotation vector components in expressions (19) and (20) after their preliminary componentwise representation. Eventually, we obtain the relations between the stiffness tensor coefficients and interaction parameters on the microscale:

$$\begin{aligned}
A_{1111} &= A_{2222} = \frac{\sqrt{3}}{6}\frac{C_A(C_A+3C_D)}{C_A+C_D},\\
C_{1111} &= C_{2222} = \frac{\sqrt{3}}{6}\frac{C_T(C_T+3C_B)}{C_T+C_B},\\
A_{1122} &= A_{2211} = \frac{\sqrt{3}}{6}\frac{C_A(C_A-C_D)}{C_A+C_D},\\
C_{1122} &= C_{2211} = \frac{\sqrt{3}}{6}\frac{C_T(C_T-C_B)}{C_T+C_B},\\
A_{1212} &= A_{2121} = \frac{\sqrt{3}}{6}\frac{C_D(C_D+3C_A)}{C_A+C_D},\\
C_{1212} &= C_{2121} = \frac{\sqrt{3}}{6}\frac{C_B(C_B+3C_T)}{C_T+C_B},\\
A_{1221} &= A_{2112} = \frac{\sqrt{3}}{6}\frac{C_D(C_A-C_D)}{C_A+C_D},\\
C_{1221} &= C_{2112} = \frac{\sqrt{3}}{6}\frac{C_B(C_T-C_B)}{C_T+C_B},\\
A_{3131} &= A_{3232} = \frac{\sqrt{3}}{3}C_D,\ \ C_{3131} = C_{3232} = \frac{\sqrt{3}}{3}C_B.
\end{aligned} \quad (24)$$

Equation (24) contains nonzero components of the tensor ${}^4\mathbf{A}$ and tensor ${}^4\mathbf{C}$. The continuum equivalent to the graphene lattice is invariant with respect to rotations about the normal $\mathbf{e}_3$ and to reflections from the basal planes. According to the Curie principle [18], the stiffness tensors are bound to have the same symmetry, as reflected in (24): only this set of nonzero components and equality of the tensor ${}^4\mathbf{B}$ to zero provides the specified symmetry. The components in (24) are not independent and some of them can be expressed in terms of the others:

$$A_{1212} + A_{1221} = A_{1111} - A_{1122},\ \ C_{1212} + C_{1221} = C_{1111} - C_{1122}. \quad (25)$$

The system of equations (24) can give one more relation:

$$A_{3131} = \frac{A_{1111}^2 - A_{1122}^2}{3A_{1122} + A_{1111}},\ \ C_{1221} = \frac{C_{1122}(C_{1111} - C_{1122})}{3C_{1122} + C_{1111}}. \quad (26)$$

The tensor ${}^4\mathbf{A}$ relates the force stress tensor $\mathbf{T}$ and the strain tensor $\boldsymbol{\varepsilon}$, and the tensor ${}^4\mathbf{C}$ relates the couple stress tensor $\mathbf{M}$ and the strain tensor $\boldsymbol{\kappa}$:

$$\begin{gathered} T_{11} = A_{1111}\varepsilon_{11} + A_{1122}\varepsilon_{22}, \\ T_{22} = A_{2211}\varepsilon_{11} + A_{2222}\varepsilon_{22}, \\ T_{21} = A_{1221}\varepsilon_{12} + A_{1212}\varepsilon_{21}, \\ T_{12} = A_{2121}\varepsilon_{12} + A_{2112}\varepsilon_{21}, \\ T_{13} = A_{3131}\varepsilon_{13},\ T_{23} = A_{3232}\varepsilon_{23}, \\ M_{11} = C_{1111}\kappa_{11} + C_{1122}\kappa_{22}, \\ M_{22} = C_{2211}\kappa_{11} + C_{2222}\kappa_{22}, \\ M_{21} = C_{1221}\kappa_{12} + C_{1212}\kappa_{21}, \\ M_{12} = C_{2121}\kappa_{12} + C_{2112}\kappa_{21}, \\ M_{13} = C_{3131}\kappa_{13},\ M_{23} = C_{3232}\kappa_{23}. \end{gathered} \tag{27}$$

The strain tensors $\boldsymbol{\varepsilon}$, $\boldsymbol{\kappa}$ have the following components:

$$\begin{gathered} \varepsilon_{11} = u^x_{,x},\ \varepsilon_{12} = u^y_{,x} - \varphi^z,\ \varepsilon_{13} = u^z_{,x} + \varphi^y,\ \varepsilon_{21} = u^x_{,y} + \varphi^z, \\ \varepsilon_{22} = u^y_{,y},\ \varepsilon_{23} = u^z_{,y} - \varphi^x,\ \kappa_{11} = \varphi^x_{,x},\ \kappa_{21} = \varphi^x_{,y}, \\ \kappa_{12} = \varphi^y_{,x},\ \kappa_{22} = \varphi^y_{,y},\ \kappa_{13} = \varphi^z_{,x},\ \kappa_{23} = \varphi^z_{,y}. \end{gathered} \tag{28}$$

Reasoning from these relations, one can define the physical meaning of different stiffness tensor components. The coefficient A_{1111} is responsible for tensile properties, A_{1122} for Poisson's effect, A_{1212} and A_{1221} for shear strain and stress in the vector plane $\mathbf{e}_1, \mathbf{e}_2$, coefficient A_{3131} for those in the orthogonal plane, C_{1111} for torsional properties, and C_{1221} for analogue of the Poisson's effect in torsion.

Let us define the bending stiffness D as a coefficient between the couple stress in a section orthogonal to $\mathbf{e}_1$ and the strain κ_{12} (or $\mathbf{e}_2$ and κ_{21}). Then, this coefficient is equal to C_{1212} (C_{2121}):

$$D = \frac{\sqrt{3}}{6}\frac{C_B(C_B + 3C_T)}{C_B + C_T}. \tag{29}$$

Unfortunately, there is a lack of experimental data to determine all elastic moduli. For this reason, let us consider a simplified theory to operate with a smaller number of independent parameters. Assume that no in-plane couple stresses are present. The stiffness tensor ${}^4\mathbf{A}$ is thus bound to be invariant with respect to transposition of a pair of indices 12 and 21. So, we can introduce a new component $A^*_{1212} = (A_{1212} + A_{1221})/2$ to fit the simplified theory as:

$$A^*_{1212} = A^*_{1221} = A^*_{2121} = A^*_{2112} = \frac{\sqrt{3}}{3}\frac{C_A C_D}{C_A + C_D}. \tag{30}$$

The results for the coefficients A_{1111} and A_{1122} descriptive of in-plane strains coincide with those obtained earlier [22] using experimental data for graphite to calculate the force constants C_A and C_D. It is found that $C_D/C_A = 0.55$ suggesting that the transverse stiffness is comparable to the longitudinal stiffness and is to be taken into account.

As can be seen from expressions (24), Poisson's effect disappears if $C_A = C_D$. The same is true at $C_T = C_B$: there is no torsion orthogonal to the direction of applied torque.

2.3. Rod Model of Carbon Bond in Graphene

By now, many efficient approaches have been proposed for microscale dynamic simulation of graphene. Among them are ab initio and molecular dynamics methods [10–17, 24] and molecular mechanics methods [25, 26]. A distinguishing feature of our approach is that we propose a quite definite mechanical model of carbon bond—an elastic rod that operates under tension-compression and bending-torsion. The rod models the interaction of electron clouds responsible for directional covalent chemical bonds. Clearly, the elastic characteristics of the rod should be chosen so that the resulting model fits experimental values of the elastic characteristics of an examined crystal. At the same time, the studies [22, 27] show that this bond can be described using the moment approach such that the characteristics of moment interaction can be determined for graphene and diamond.

For better understanding, let us dwell on the basic equations of the linear theory of rods [26] and on some problems the solution of which are required in our further consideration. Let the displacements of rod points be described by the equations:

$$\mathbf{u} = u\mathbf{t} + \mathbf{w},\ \mathbf{t}\cdot\mathbf{w} = 0,\ \boldsymbol{\psi} = \psi\mathbf{t} + \mathbf{t}\times\boldsymbol{\theta},\ \boldsymbol{\theta}\cdot\mathbf{t} = 0. \tag{31}$$

Here u is the longitudinal displacement of rod points, $\mathbf{w}$ is the transverse displacement vector, ψ is torsion, $\mathbf{t}$ is the unit tangent vector. The strain vectors are given by the relations

$$\mathbf{e} = \varepsilon\mathbf{t} + \boldsymbol{\gamma},\ \varepsilon = u',\ \boldsymbol{\gamma} = \mathbf{w}' - \boldsymbol{\theta},\ \boldsymbol{\varphi} \approx \psi'\mathbf{t} + \mathbf{t}\times\boldsymbol{\theta}'. \tag{32}$$

Here ε is the elongation of the rod, $\boldsymbol{\gamma}$ is the transverse shear strain vector, ψ' is the torsion of the rod, $\boldsymbol{\theta}$ is the bending strain vector.

In the linear theory of rods without natural torsion, the relations for forces and moments acting in the rod take the form:

$$\begin{gathered} \mathbf{n} = \tilde{\mathbf{A}}\cdot\mathbf{e},\ \mathbf{m} = \tilde{\mathbf{C}}\cdot\boldsymbol{\varphi},\ \mathbf{n} = T\mathbf{t} + \mathbf{q}, \\ \mathbf{t}\cdot\mathbf{q} = 0,\ \mathbf{m} = H\mathbf{t} + \mathbf{t}\times\mathbf{l},\ \mathbf{t}\cdot\mathbf{l} = 0. \end{gathered} \tag{33}$$

Here T is the longitudinal force in the rod, H is the torque, $\mathbf{q}$ is the transverse force vector, $\mathbf{l}$ is the bending moment vector.

The stress tensors $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{C}}$ are expressed as follows:

$$\tilde{\mathbf{A}} = EF\mathbf{tt} + kGF(\mathbf{E} - \mathbf{tt}),\ \ \tilde{\mathbf{C}} = GJ_r\mathbf{tt} + E\,{}^2\mathbf{c},$$
$$^2\mathbf{c} = J_1\mathbf{d}_1\mathbf{d}_1 + J_2\mathbf{d}_2\mathbf{d}_2,\ \ k = \pi^2/12. \tag{34}$$

In the above formulae, E is Young's modulus, F is the cross-sectional area of the rod, G is the shear modulus, k is the transverse shear coefficient, $\mathbf{d}_1$ and $\mathbf{d}_2$ are the normal and binormal vectors, J_1 and J_2 are the respective inertia moments for the rod cross-section. The quantity J_r stands for the geometric torsional stiffness such that J_r for an elliptical rod is equal to the polar moment of inertia J_p.

Using the above notation with neglecting distributed external forces and moments, the equilibrium equations for the rod can be represented as:

$$\mathbf{n}'(s) = 0,\ \ \mathbf{m}'(s) + \mathbf{t}\times\mathbf{n}(s) = 0, \tag{35}$$

where s is the natural coordinate of the rod.

Let us consider a system of two particles, of which one is rigidly fixed and the other is displaced relative to it by a translation vector $\mathbf{u}^*$ and rotation vector $\boldsymbol{\varphi}^*$. So the particles, according to the moment approach, start experience force and moment interactions (7) characterized by the components C_A, C_B, C_T, and C_D. On the other hand, it can be assumed that the particles are connected via an elastic rod whose left end is fixed and right end is shifted from the equilibrium position by a vector $\mathbf{u}^*$ and rotated through an angle $\boldsymbol{\varphi}^*$. As a result, forces dependent on $\mathbf{u}^*$ and $\boldsymbol{\varphi}^*$ arise in the rod. Static equations (35) for them give

$$\mathbf{n} = \mathbf{n}_0 = \text{const},\ \ \mathbf{m} = \mathbf{m}_0 - \mathbf{t}\times\mathbf{n}_0 s. \tag{36}$$

Let us introduce, in view of (36), the following notation for the force and moment at the rod end:

$$\mathbf{n}^* = \mathbf{n}_0 = \text{const},\ \ \mathbf{m}^* = \mathbf{m}_0 - \mathbf{t}\times\mathbf{n}_0 l. \tag{37}$$

On the other hand, according to (33), we have

$$\mathbf{n} = \tilde{\mathbf{A}}\cdot(\mathbf{u}' + \mathbf{t}\times\boldsymbol{\varphi}),\ \ \mathbf{m} = \tilde{\mathbf{C}}\cdot\boldsymbol{\varphi}'. \tag{38}$$

Simultaneous solution of (36) and (38) gives us the expression for displacement and rotation vectors:

$$\mathbf{u} = \tilde{\mathbf{A}}^{-1}\cdot\mathbf{n}_0 s - \mathbf{t}$$
$$\times(\tilde{\mathbf{C}}^{-1}\cdot(1/2\,\mathbf{m}_0 s^2 - 1/6\,\mathbf{t}\times\mathbf{n}_0 s^3) + \boldsymbol{\varphi}_0 s) + \mathbf{u}_0, \tag{39}$$
$$\boldsymbol{\varphi} = \tilde{\mathbf{C}}^{-1}\cdot(\mathbf{m}_0 s - 1/2\,\mathbf{t}\times\mathbf{n}_0 s^2) + \boldsymbol{\varphi}_0.$$

In view of the boundary conditions

$$\mathbf{u}\big|_{s=0} = 0,\ \ \boldsymbol{\varphi}\big|_{s=0} = 0,\ \ \mathbf{u}\big|_{s=l} = \mathbf{u}^*,\ \ \boldsymbol{\varphi}\big|_{s=l} = \boldsymbol{\varphi}^*, \tag{40}$$

we find that

$$\mathbf{u}_0 = 0,\ \ \boldsymbol{\varphi}_0 = 0,$$
$$\boldsymbol{\varphi}^* = \tilde{\mathbf{C}}^{-1}\cdot(\mathbf{m}_0 l - 1/2\,\mathbf{t}\times\mathbf{n}_0 l^2), \tag{41}$$
$$\mathbf{u}^* = \tilde{\mathbf{A}}^{-1}\cdot\mathbf{n}_0 l - \mathbf{t}\times(\tilde{\mathbf{C}}^{-1}\cdot(1/2\,\mathbf{m}_0 l^2 - 1/6\,\mathbf{t}\times\mathbf{n}_0 l^3)).$$

Let us solve (37) and (41) for $\mathbf{u}^*$ and $\boldsymbol{\varphi}^*$. So, the force acting at the rod end can be reduced to the form:

$$\mathbf{n}^* = \mathbf{A}\cdot\boldsymbol{\varepsilon}^*,\ \ \boldsymbol{\varepsilon}^* = \mathbf{u}^* + 1/2\,\mathbf{t}\times\boldsymbol{\varphi}^*,$$
$$\mathbf{A} = (\tilde{\mathbf{A}}^{-1} - 1/12\,(\mathbf{t}\times\tilde{\mathbf{C}}^{-1}\times\mathbf{t})l^3)^{-1}. \tag{42}$$

Comparison of the latter relations with (7)–(10) shows that we have managed to derive the same form of interaction force as that obtained in the discrete approach. The tensor components $\mathbf{A}$ can be found by expressing the second rank tensor as

$$\boldsymbol{\Lambda} = \lambda_1\mathbf{tt} + \lambda_2\mathbf{d}_1\mathbf{d}_1 + \lambda_1\mathbf{d}_2\mathbf{d}_2. \tag{43}$$

It is easy to check that the inverse tensor, in this case, has the form:

$$\boldsymbol{\Lambda}^{-1} = 1/\lambda_1\,\mathbf{tt} + 1/\lambda_2\,\mathbf{d}_1\mathbf{d}_1 + 1/\lambda_1\,\mathbf{d}_2\mathbf{d}_2. \tag{44}$$

By using this and by substituting expressions (34), we can find the components of interest:

$$C_A = \mathbf{t}\cdot\mathbf{A}\cdot\mathbf{t} = EF/l,$$
$$C_D = \mathbf{d}_1\cdot\mathbf{A}\cdot\mathbf{d}_1 = \frac{12kEJ_2F}{kFl^3 + 24J_2(1+\nu)l}. \tag{45}$$

The equations of the theory of rods used by us to derive (45) take into account transverse shear strains and correspond to the Timoshenko beam model. This model allows the use of Poisson's ratio ν as an independent parameter in the expression for C_D. However, if there is no need to account for transverse shear, one can use a simpler model, e.g., the Bernoulli–Euler model. To switch to the latter model, we can put $k \to \infty$ in (45). Then, we obtain

$$C_A = \frac{EF}{l},\ \ C_D = \frac{12EJ_2}{l^3}. \tag{46}$$

The moment at the rod end can be expressed in a form similar to (11):

$$\mathbf{m}^* = \boldsymbol{\varepsilon}_1^*\cdot\tilde{\tilde{\mathbf{B}}} + \tilde{\tilde{\mathbf{C}}}\cdot\boldsymbol{\kappa}_1^*, \tag{47}$$

where

$$\tilde{\tilde{\mathbf{B}}} = 1/2\,\mathbf{t}\times\mathbf{A},\ \ \tilde{\tilde{\mathbf{C}}} = 1/l\,\tilde{\mathbf{C}} - 1/4\,\mathbf{t}\times\mathbf{A}\times\mathbf{t}l^2,$$
$$\boldsymbol{\varepsilon}_1^* = \mathbf{u} + (\mathbf{t}\times\boldsymbol{\varphi}^*)l,\ \ \boldsymbol{\kappa}_1^* = \boldsymbol{\varphi}^*. \tag{48}$$

Using (11), it is easy to verify that the bending stiffness C_B can be found by the formula:

$$C_B = 1/l\,\mathbf{d}_2\cdot\tilde{\mathbf{C}}\cdot\mathbf{d}_2 = (EJ_2)/l. \tag{49}$$

Noteworthy is that expressions (48) can easily give the torsional stiffness of an elastic rod about its axis, which is not considered in our moment approach:

$$C_T = 1/l\,\mathbf{t}\cdot\tilde{C}\cdot\mathbf{t} = (GJ_r)/l. \tag{50}$$

2.4. Bending Stiffness of a Graphene Sheet

Let us model the bond between two lattice atoms by linear elastic rods. For definiteness we assume that the

rods are round, their diameter is constant, and their length is equal to the interatomic bond length. Then, the area, the moment of inertia of the rod section, and the polar moment of inertia take the respective forms:

$$F = \frac{\pi d^2}{4},\ J_2 = \frac{\pi d^4}{64},\ J_\mathrm{p} = \frac{\pi d^4}{64}. \qquad (51)$$

Here d is the rod diameter. Let us determine the elastic characteristics of the rods using the Euler model. From (46), in view of (51), we can obtain the expressions for Young's modulus and diameter in terms of longitudinal and transverse bond stiffnesses:

$$E = \frac{3C_A^{\,2}}{\pi l C_D},\ d = \frac{2\sqrt{3}}{3}\sqrt{\frac{C_D}{C_A}}\,l, \qquad (52)$$

which completely determine the elastic properties of the rods in the model.

Substitution of (51), (52) in (49) and (50) can give us the expression for the bending and torsional stiffnesses of the rods:

$$C_B = \frac{C_A d^2}{16} = \frac{C_D l^2}{12},\ C_T = \frac{C_A d^2}{16(1+\nu)} = \frac{C_D l^2}{12(1+\nu)}. \qquad (53)$$

Substitution of (53) in (29) gives the expression for the bending stiffness of a graphene sheet:

$$D = \frac{\sqrt{3}}{48}\kappa(\nu) C_A d^2 = \frac{\sqrt{3}}{36}\kappa(\nu) C_D a^2, \qquad (54)$$

$$\kappa(\nu) = \frac{4+\nu}{4+2\nu}.$$

The bending stiffness contains an independent parameter—Poisson's ratio—which, generally speaking, remains undetermined. For this parameter, there is a limitation $-1.0 \le \nu < 0.5$ which gives

$$9/10 \le \kappa(\nu) \le 3/2. \qquad (55)$$

The parameters C_A and C_D can be uniquely determined from the elastic characteristics of a material. In particular for graphene, according to [22], these characteristics can be found using the experimental data of [3]:

$$C_A = 730.2\ \text{N/m},\ C_D = 401.6\ \text{N/m},\ l = 0.142\ \text{nm}. \qquad (56)$$

Then, substitution of (55), (56) in (54) gives

$$0.35 \le D \le 0.58\ \text{nN}\cdot\text{nm}. \qquad (57)$$

3. DISCUSSION OF THE RESULTS AND CONCLUDING REMARKS

Thus, our calculations allow one to determine the bending stiffness of a graphene sheet through modeling the carbon bond by rods bent according to the Bernoulli–Euler model. However, this approach has a significant drawback.

Substitution of (56) in (52) gives $E = 8.928$ TPa, $d = 0.122$ nm; that is the rod diameter compares with the rod length and a significant error may arise in estimating the bending by the Bernoulli–Euler model. It would be more appropriate to use the Timoshenko model; however, in this case, there appears one more undetermined parameter—the transverse shear coefficient k. Generally speaking, this coefficient depends on the cross-section shape. For rods and shells, the passage from theories that account for shear to classical theories is through the limit $k \to \infty$. In the theory of shells with regard to shear, one can show that the parameter k lies in the range $\pi^2/12 \le k \le 1$ [28]. However, in the theory of rods this fact is unproven [29], and therefore, due to specificity of the model material, we leave this parameter without its upper bound.

From (46) it follows that

$$\frac{C_A}{C_D} = \frac{4}{3}\frac{L^2}{d^2} + \frac{2(1+\nu)}{k}. \qquad (58)$$

Because the rod diameter and length are positive, we can relate Poisson' ratio and transverse shear coefficient as

$$-1 < \nu < \frac{kC_A}{2C_D} - 1. \qquad (59)$$

From this it follows that $k > 2C_D/C_A$ at $\nu = 0$, and the k dependence of d is thus a rapidly decreasing monotonic function.

At $k = 2C_D/C_A$, the rod diameter tends to infinity, and its minimum value is reached at $k \to \infty$ and is equal to $d = 0.122$ nm given by classical theories. At $k = 4.12$, the rod length becomes comparable to the rod diameter, and the bending stiffness is 0.53 nN·nm. At $k = 10$, the rod diameter differs by less than 5% from that given by the classical theory.

If we use the classical value of the transverse shear coefficient and put $k = \pi^2/12$, condition (59) that provides positive diameters of the rod material simulative of the carbon bond gives the following interval of possible values of Poison's ratio:

$$-1 < \nu < -0.252. \qquad (60)$$

Note that at $\nu \to -0.252$, the rod diameter increases without limit, and at $\nu \to -1$, the bending stiffness becomes equal to that obtained earlier using the Bernoulli–Euler model (0.122 nm).

Thus, the approach proposed in the paper makes it possible to determine the elastic characteristics of graphene. The graphene lattice is modeled by a set of body-points interacting with each other via forces and moments. These interactions are characterized by micro-scale force constants. The energy approach used to identify the elastic strain energy of a unit lattice cell with the elastic strain energy of its equivalent continuum allows deriving the relation between the force constants (micro-scale parameters) and the elastic moduli of the conti-

nuum (macroscale parameters). One of the macroscale characteristics of particular interest is bending stiffness. In the paper, this parameter is defined as the proportionality factor between the components of the couple stress tensor and torsional strains corresponding to bending strains. The analytical dependences obtained for the microscale interaction parameters and macroscale parameters of the material allow one to obtain expressions for the bending stiffness and for other elastic characteristics. However, to do this requires estimation of the microscale parameters (torsional and bending stiffnesses of the bond), for example, from experimental data or from data used to determine the parameters of distributed force fields for graphite structures. At present, there are difficulties in experimental determination of the torsional and bending stiffnesses of covalent bonds in graphene. Therefore, it is proposed to use some additional assumptions on the bond between atoms by applying the rod model. The model allows expressing the bending stiffness of graphene in terms of transverse and longitudinal stiffnesses responsible for in-plane strains of a graphene sheet. These stiffnesses can be determined from the available experimental data for graphite. As a result, we obtain the bending stiffness of a graphene sheet. The obtained analytical values of the bending stiffness have the same order of magnitude as those given by computer simulation based on empirical potentials and ab initio calculations.

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