Description of equivalent elastic continuum for graphene lattice

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Abstract

The work contributes to the study of equivalent continuum model that is able to describe the elastic moduli of graphene — monolayer of carbon atoms. The moment interaction between the particles that form the lattice is described by four force constants and depends on the position of particles and their orientation in space. An approach is applied to link the macroscopic moduli and the parameters of interaction at microlevel based on the comparison of the energy of the microstructure and the energy of the equivalent continuous plate. The comparison with structural mechanics approach is carried out and the elastic moduli are derived for the parameters of interaction taken from AMBER force field.

1   Introduction

Graphene is the mother structure of most carbon based materials. A single 2-D sheet of graphene is a hexagonal structure with each carbon atom forming three bonds with its nearest neighbours. In the last decade the enhanced attention has been paid to the study of this material due to its unique properties found (e.g. high conductivity, extremely high strength) and the recent possibility to extract a layer of graphene one atom thick. This has induced the development of theoretical models for graphene as well as the experimental study. The combination of atomistic simulations and continuum elasticity focuses on graphene mechanical properties, especially as for the elastic moduli. The experimental studies of graphene membranes suspended on a silicon substrate with holes has been carried out using atomic force microscope [1]–[3]. The Young Modulus of graphene sheet has been found to be around 350 N/m. As for other elastic moduli, there is still a lack of experimental data.

Different approaches are applied to build analytical models for analysis of carbon structures. The empirical force field models are widely used to describe the mechanical behaviour of the systems containing significant number of atoms [4]. In [5]–[6] such models are proposed based on the parametric many-body potentials for carbon structures [7]–[8] and the elastic moduli are evaluated for the equivalent continuum. The mechanical properties of graphene have been derived from the first principles in [9] – [11]. An equivalent continuum model was proposed in [12]–[14]. In [15]–[16] the molecular model based on AMBER force field constants of interaction for covalent bonds has been linked with the space-frame structural mechanics model and FEM simulations have been carried out. However, there is a huge scattering of the results of theoretical studies. The number of parameters of interatomic potentials used in the studies is relatively large and the meaning of these parameters often remains obscure. Such potentials are usually unable to satisfy all elastic constants of the described material. Three-particle interaction, special case of many-body potential, has been considered in [17]. The effective force constants of interaction have been evaluated from the experimental data to provide exact matching in case of in-plane deformation of graphene.

Covalent bond is a directional bond. This can be allowed for by taking into account a so called moment contribution to the interatomic interaction as an alternative to many-body potential models where the potential energy is a function of the positions of N particles regarded as material points. This contribution is usually implicitly considered when torsional and bending properties

of a bond are taken into account (for example, when a bond is modelled as a beam). In [18] it was proposed to represent a particle in the lattice as a set of material points rigidly connected to each other. The interaction between material points from different sets is described by pairwise potential. As the result the moment component of interaction between the particles is present introducing additional transversal stiffness. Another way to account for the moment interaction at microlevel in an explicit form is to consider rotational degrees of freedom of particles forming the lattice. This approach is described in [19] where the relation between constants of interaction and the elastic moduli of in-plane deformation of graphene lattice are obtained. In this paper the latter approach is applied to derive the equivalent continuum able to describe also out-of-plane deformations of graphene. The material is represented as a set of particles (solids) which interact in terms of forces and torques. A method based on the energies equivalence is applied to obtain the relations between the constants of interaction at microlevel and elastic moduli of continuum corresponding to the discrete structure of graphene.

2   Interatomic potential

The discrete structure of a material is presented as a set of particles with three translational and three rotational degrees of freedom. The interaction between nearest neighbours is taken into account. The bonds between the particles are assumed to be transversely-isotropic for the sake of simplicity. Four force constants are proposed to describe the deformation of a bond: A_1 is the bond stretching resistance force constant, A_2 describes the resistance to shear deformations, C_1 — to torsion, C_2 — to bending of the bond. Potential energy of elastic deformation of a crystal structure per unit cell can be presented as a sum of potential energies of deformation of the bonds between some reference particle in the cell and its nearest neighbours:

$$W = \frac{1}{2V_0} \sum_\alpha \Pi_\alpha, \tag{1}$$

where Π_α is a potential of interaction between the particle in the cell and its neighbour with index α, V_0 is a volume per particle in the unit cell of the lattice. In general, there can be more than one particle in the unit cell, lattice with one particle in the unit cell is called simple and otherwise complex. The lattice of graphene contains two particles per unit cell and thus is complex. It consists of two triangular sublattices. The potential Π_α can be presented as a quadratic form of strain vectors and stiffness tensors of the bond

$$\Pi_\alpha = \frac{1}{2}\varepsilon_\alpha \cdot \underline{\underline{A}}_\alpha \cdot \varepsilon_\alpha + \varepsilon_\alpha \cdot \underline{\underline{B}}_\alpha \cdot \kappa_\alpha + \frac{1}{2}\kappa_\alpha \cdot \underline{\underline{C}}_\alpha \cdot \kappa_\alpha. \tag{2}$$

Here $\underline{\underline{A}}_\alpha$, $\underline{\underline{B}}_\alpha$, $\underline{\underline{C}}_\alpha$ are stiffness tensors of the bond α and they contain information about the deformation of the bond in different directions:

$$\begin{aligned}
\underline{\underline{A}}_\alpha &= A_1 \underline{n}_\alpha \underline{n}_\alpha + A_2 \left(\underline{\underline{E}} - \underline{n}_\alpha \underline{n}_\alpha \right), \\
\underline{\underline{C}}_\alpha &= C_1 \underline{n}_\alpha \underline{n}_\alpha + C_2 \left(\underline{\underline{E}} - \underline{n}_\alpha \underline{n}_\alpha \right), \qquad a\underline{n}_\alpha = \underline{a}_\alpha,
\end{aligned} \tag{3}$$

tensor $\underline{\underline{B}}$ is equal to zero if a lattice has two normal to each other planes of symmetry [20]. It holds true in case of graphene lattice. Vector $\underline{a}_\alpha$ connects two neighbour particles, a is a length of a bond in equilibrium configuration, $\underline{\underline{E}}$ is a unit tensor; ε_α, κ_α are strain vectors and are expressed as follows [20]:

$$\varepsilon_\alpha = \underline{u}_\alpha - \underline{u} + \frac{1}{2}\underline{a}_\alpha \times (\underline{\varphi}_\alpha + \underline{\varphi}), \qquad \kappa_\alpha = \underline{\varphi}_\alpha - \underline{\varphi}. \tag{4}$$

Here $\underline{u}_\alpha$, $\underline{u}$, $\underline{\varphi}_\alpha$, $\underline{\varphi}$ are translations and rotations of the particle with index α and some reference particle relative to their equilibrium position.

Equations (2) – (4) are substitutted into (1) and thus the potential energy of the system of particles is obtained depending on position of particles $\underline{u}$, $\underline{u}_\alpha$, orientation $\underline{\varphi}$, $\underline{\varphi}_\alpha$, geometry of initial configuration $\underline{a}_\alpha$ and constants of interaction A_1, A_2, C_1, C_2.

3   Towards the macroscale

Let us confront the displacements and rotations of the particles with the displacements and rotations of continuum $\underline{u} = \underline{u}(\underline{r})$, $\underline{\varphi} = \underline{\varphi}(\underline{r})$, where $\underline{r}$ is radius-vector in initial configuration. Then displacements and rotations of neighbour particles are $\underline{u}_\alpha = \underline{u}(\underline{r} - \underline{a}_\alpha)$, $\underline{\varphi}_\alpha = \underline{\varphi}(\underline{r} - \underline{a}_\alpha)$. Under long-wave approximation[2] these displacement and rotations can be expressed as follows:

$$\underline{u}_\alpha = \underline{u} + \underline{a}_\alpha \cdot \nabla \underline{u} + \eta \underline{\zeta}, \qquad \underline{\varphi}_\alpha = \underline{\varphi} + \underline{a}_\alpha \cdot \nabla \underline{\varphi} + \eta \underline{\psi}, \tag{5}$$

where ∇ is the nabla operator. Parameter η is equal to 1 for lattices that contain two atoms in the unit cell (complex lattice) and to 0 if there is only one atom in the unit cell of the lattice (simple lattice). Vectors $\underline{\zeta}$, $\underline{\psi}$ denote relative displacements and rotations of the particles from different sublattices constitutting complex lattice.

Equations (5) can be substitutted in the energy W derived in the previous section. Vectors $\underline{\zeta}$, $\underline{\psi}$ correspond to the minimum of potential energy of the lattice and thus can be found from the system of equations

$$\frac{\partial W}{\partial \underline{\zeta}} = 0, \qquad \frac{\partial W}{\partial \underline{\psi}} = 0. \tag{6}$$

Finally, the energy of the corresponding continuum W can be obtained:

$$W = W(\nabla \underline{u}, \nabla \underline{\varphi}, \underline{\varphi}, A_1, A_2, C_1, C_2). \tag{7}$$

It can be also presented as a quadratic form of stiffness tensors of fourth rank and strain tensors:

$$W = \frac{1}{2}\underline{\underline{\varepsilon}} \cdot \cdot {}^4\underline{\underline{A}} \cdot \cdot \underline{\underline{\varepsilon}} + \underline{\underline{\varepsilon}} \cdot \cdot {}^4\underline{\underline{B}} \cdot \cdot \underline{\underline{\kappa}} + \frac{1}{2}\underline{\underline{\kappa}} \cdot \cdot {}^4\underline{\underline{C}} \cdot \cdot \underline{\underline{\kappa}}. \tag{8}$$

Strain tensors are

$$\underline{\underline{\varepsilon}} = \nabla \underline{u} + \underline{\underline{E}} \times \underline{\varphi}, \qquad \underline{\underline{\kappa}} = \nabla \underline{\varphi}. \tag{9}$$

In order to obtain the relations between coefficients of stiffness tensors at macrolevel and force constants of interaction at microlevel the representations (7) and (8) should be compared.

4   The lattice of graphene

The lattice of graphene is 2D lattice where carbon atoms are located in the nodes of hexagons. Let us introduce orthonormal basis $\{\underline{e}_1, \underline{e}_2, \underline{e}_3\}$, where $\underline{e}_1$ and $\underline{e}_2$ lie in the plane, $\underline{e}_3$ is normal to the plane containing the lattice. Let us name the axes with the unit vectors $\underline{e}_1$, $\underline{e}_2$, $\underline{e}_3$ as x, y and z, respectively. The vectors $\underline{u}$, $\underline{\varphi}$, $\underline{a}_\alpha$ can be expressed then

$$\underline{u} = u^x(x,y)\underline{e}_1 + u^y(x,y)\underline{e}_2 + u^z(x,y)\underline{e}_3,$$
$$\underline{\varphi} = \varphi^x(x,y)\underline{e}_1 + \varphi^y(x,y)\underline{e}_2 + \varphi^z(x,y)\underline{e}_3, \tag{10}$$

and vectors $\underline{a}_\alpha$ are

$$\underline{a}_1 = \underline{e}_1, \quad \underline{a}_2 = -\frac{1}{2}\underline{e}_1 + \frac{\sqrt{3}}{2}\underline{e}_2, \quad \underline{a}_3 = -\frac{1}{2}\underline{e}_1 - \frac{\sqrt{3}}{2}\underline{e}_2. \tag{11}$$

Derivation of the relations between the coefficients of the stiffness tensors of corresponding continuum and parameters of interactions at microlevel is carried out by comparing the multipliers of similar terms of $u^x_{,x}$, $u^x_{,y}$, $u^y_{,x}$, $u^y_{,y}$, $u^z_{,y}$, $u^z_{,x}$, $\varphi^x_{,x}$, $\varphi^x_{,y}$, $\varphi^y_{,x}$, $\varphi^y_{,y}$, $\varphi^z_{,x}$, $\varphi^z_{,y}$, φ_x, φ_y, φ_z in (7) and (8).

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[2]The expansion is valid for the waves with lengthes far larger than interatomic distance a_α in initial configuration which is assumed to be a small parameter.

A comma stands for the first derivative with respect to the coordinate that follows. Finally, the coefficients of the stiffness tensors $^4\underline{\underline{A}}$, $^4\underline{\underline{C}}$ are expressed as:

$$A_{1111} = A_{2222} = \frac{\sqrt{3}}{6}\frac{A_1(A_1+3A_2)}{A_1+A_2}, \quad C_{1111} = C_{2222} = \frac{\sqrt{3}}{6}\frac{C_1(C_1+3C_2)}{C_1+C_2};$$

$$A_{1122} = A_{2211} = \frac{\sqrt{3}}{6}\frac{A_1(A_1-A_2)}{A_1+A_2}, \quad C_{1122} = C_{2211} = \frac{\sqrt{3}}{6}\frac{C_1(C_1-C_2)}{C_1+C_2};$$

$$A_{1212} = A_{2121} = \frac{\sqrt{3}}{6}\frac{A_2(A_2+3A_1)}{A_1+A_2}, \quad C_{1212} = C_{2121} = \frac{\sqrt{3}}{6}\frac{C_2(C_2+3C_1)}{C_1+C_2}; \tag{12}$$

$$A_{1221} = A_{2112} = \frac{\sqrt{3}}{6}\frac{A_2(A_1-A_2)}{A_1+A_2}, \quad C_{1221} = C_{2112} = \frac{\sqrt{3}}{6}\frac{C_2(C_1-C_2)}{C_1+C_2};$$

$$A_{3131} = A_{3232} = \frac{\sqrt{3}}{3}A_2, \qquad\qquad C_{3131} = C_{3232} = \frac{\sqrt{3}}{3}C_2.$$

The left column shows nonzero components of tensor $^4\underline{\underline{A}}$ and the right one — of tensor $^4\underline{\underline{C}}$. The obtained equivalent plate is invariant to the rotation around its normal $\underline{e}_3$ and reflection from itself and from two mutually orthogonal planes. This leads to the same symmetry of stiffness tensors due to Curie's Principle and this symmetry is reflected in the results (12) [21]. The relation between some of the components takes place due to the mentioned isotropy:

$$A_{1212} + A_{1221} = A_{1111} - A_{1122}, \qquad C_{1212} + C_{1221} = C_{1111} - C_{1122}. \tag{13}$$

Another relation can be derived from the system of equations (12):

$$A_{3131} = \frac{A_{1111}^2 - A_{1122}^2}{3A_{1122} + A_{1111}}, \qquad C_{1221} = \frac{C_{1122}(C_{1111} - C_{1122})}{3C_{1122} + C_{1111}}. \tag{14}$$

All the components of tensor $^4\underline{\underline{B}}$ turned out to be zero — this can also be predicted by applying the theory of symmetry [21]. Tensor $^4\underline{\underline{A}}$ provides a relation between stress tensor $\underline{T}$ and strain tensor $\underline{\varepsilon}$ and tensor $^4\underline{\underline{C}}$ — between couple stress tensor $\underline{M}$ and strains $\underline{\kappa}$:

$$T_{11} = A_{1111}\varepsilon_{11} + A_{1122}\varepsilon_{22}, \quad T_{22} = A_{2211}\varepsilon_{11} + A_{2222}\varepsilon_{22}, \quad T_{21} = A_{1221}\varepsilon_{12} + A_{1212}\varepsilon_{21}$$

$$T_{12} = A_{2121}\varepsilon_{12} + A_{2112}\varepsilon_{21}, \quad T_{13} = A_{3131}\varepsilon_{13}, \qquad\qquad T_{23} = A_{3232}\varepsilon_{23}$$

$$M_{11} = C_{1111}\kappa_{11} + C_{1122}\kappa_{22}, \quad M_{22} = C_{2211}\kappa_{11} + C_{2222}\kappa_{22}, \quad M_{21} = C_{1221}\kappa_{12} + C_{1212}\kappa_{21} \tag{15}$$

$$M_{12} = C_{2121}\kappa_{12} + C_{2112}\kappa_{21}, \quad M_{13} = C_{3131}\kappa_{13}, \qquad\qquad M_{32} = C_{3232}\kappa_{23}.$$

The components of strain tensors $\underline{\varepsilon}$, $\underline{\kappa}$ are:

$$\varepsilon_{11} = u_{,x}^x, \quad \varepsilon_{12} = u_{,x}^y - \varphi^z, \quad \varepsilon_{13} = u_{,x}^z + \varphi^y, \quad \varepsilon_{21} = u_{,y}^x + \varphi^z,$$

$$\varepsilon_{22} = u_{,y}^y, \quad \varepsilon_{23} = u_{,y}^z - \varphi^x, \quad \kappa_{11} = \varphi_{,x}^x, \qquad \kappa_{21} = \varphi_{,y}^x, \tag{16}$$

$$\kappa_{12} = \varphi_{,x}^y, \quad \kappa_{22} = \varphi_{,y}^y, \qquad \kappa_{13} = \varphi_{,x}^z, \qquad \kappa_{23} = \varphi_{,y}^z.$$

The components of the stiffness tensors have the following physical meaning: A_{1111} describes the stretching properties of the material, A_{1122} — the Poisson effect, A_{1212} and A_{1221} relate shear strains and stresses in the plane determined by vectors $\underline{e}_1$, $\underline{e}_2$ and A_{3131} — in orthogonal plane. C_{1111} describes torsion properties of the material, C_{1221} — analogue of Poisson effect in case of torsions. Let us define bending stiffness of the material D as a coefficient between couple stress in a section orthogonal to $\underline{e}_1$ and strain κ_{12} (or $\underline{e}_2$ and κ_{21}). This coefficient is equal to C_{1212} (or C_{2121}):

$$D = \frac{\sqrt{3}}{6}\frac{C_2(C_2+3C_1)}{C_1+C_2}. \tag{17}$$

There is a lack of experiments to determine all of the macroscopic moduli. In order to reduce the number of independent macroscopic moduli a simpler theory can be taken into consideration. Due to the momentless (symmetric) theory the in-plane moduli of tensor $^4\underline{\underline{A}}$ should be invariant to transposition of the pairs of indices 12 and 21. For this purpose a new component A^*_{1212} corresponding to the simpler theory should be taken as $(A_{1212} + A_{1221})/2$:

$$A^*_{1212} = A^*_{1221} = A^*_{2121} = A^*_{2112} = \frac{\sqrt{3}}{3}\frac{A_1 A_2}{A_1 + A_2}. \tag{18}$$

The results for coefifcents A_{1111} and A_{1122} that describe in-plane deformation correspond with the results obtained in [19] where experimental data for bulk graphite was applied to find the values of force constants A_1 and A_2. It turned out that $A_2/A_1 = 0.55$: transversal stiffness of covalent bond is the same order as longitudinal one and thus needs to be taken into account. The analysis of relations (18) shows that the Poisson effect is eliminated when $A_1 = A_2$. The same phenomenon takes place in case of equality of torsion and bending stiffnesses C_1 and C_2: there is no twisting in the direction orthogonal to the direction where twisting moment is applied.

5 Comparison with the structural mechanics approach

The method of the linkage of molecular mechanics and structural mechanics was proposed in [16]–[15] to use the AMBER force field [22] for the simulation of covalent bonds. From the viewpoint of molecular mechanics carbon structure can be regarded as a large molecule consisting of carbon atoms. The interactions between the atoms can be described by some force field. The representation of this field as a sum of potential energies that correspond to different interactions is widely used in literature:

$$U = \sum U_r + \sum U_\theta + \sum U_\varphi + \sum U_\omega + \sum U_{vdw}. \tag{19}$$

Here U_r corresponds to a bond stretching, U_θ is for bond angle bending, U_φ — dihedral angle torsion, U_ω — out-of-plane torsion, U_{vdw} — nonbonded van der Waals interaction. For covalent systems the main contribution comes from the first four terms which include four-body potentials. Under assumption of small deformations the simplest harmonic forms of the energies can be considered. The third and the fourth terms are usually merged to a single equivalent term U_τ. After that three harmonic forms are left:

$$U_r = \frac{1}{2}k_r(\Delta r)^2, \qquad U_\theta = \frac{1}{2}k_\theta(\Delta\theta)^2, \qquad U_\tau = \frac{1}{2}k_\tau(\Delta\varphi)^2, \tag{20}$$

where k_r, k_θ, k_τ are force constants and Δr, $\Delta\theta$, $\Delta\varphi$ are corresponding strains.

In [15] it is assumed that carbon-carbon bond can be simulated by uniform round beam-like element with parameters EI, EA and GJ, where E is the Young modulus of a beam, I is the moment of inertia J is the polar moment of inertia, G is the shear modulus, A is the cross-section area. This parameters are determined by comparing the energies of the deformation of a bond subjected to pure axial force, to pure bending moment and pure torsion:

$$U_A = \frac{1}{2}\frac{EA}{L}(\Delta L)^2, \qquad U_M = \frac{1}{2}\frac{EI}{L}(2\alpha)^2, \qquad U_T = \frac{1}{2}\frac{GJ}{L}(\Delta\beta)^2. \tag{21}$$

It is taken into account that each energy term in (20) represents individual interaction without cross-interactions and that's why strain energies of structural element under individual forces are considered. L is the length of a beam and is assumed to be equal to 0.142 nm — the length of a covalent bond in graphene. By assuming the equivalences

$$\Delta L \iff \Delta r, \qquad 2\alpha \iff \Delta\theta, \qquad \Delta\beta \iff \Delta\varphi \tag{22}$$

and comparing (20) to (21) the following relations are obtained:

$$\frac{EA}{L} = k_r, \qquad \frac{EI}{L} = k_\theta, \qquad \frac{GJ}{L} = k_\tau. \tag{23}$$

The values for k_r, k_θ, k_τ taken from the AMBER force field [22] are:

$$k_r = 6.52 \cdot 10^{-7} \text{N nm}^{-1}, \qquad k_\theta = 8.76 \cdot 10^{-10} \text{N nm rad}^{-2},$$

$$k_\tau = 2.78 \cdot 10^{-10} \text{N nm rad}^{-2}.$$

(24)

The stiffnesses A_1, A_2, C_1, C_2 can be linked with parameters of the beams and thus with force field constants. For Bernoully-Euler beam the relations between the stiffness constants and parameters of a beam are:

$$A_1 = \frac{EA}{L}, \qquad C_2 = \frac{EI}{L}, \qquad C_1 = \frac{GJ}{L}, \qquad A_2 = \frac{12EI}{L^3}.$$

(25)

Comparing (23) and (25) and taking into account (24) the following values for the stiffness coefficients are obtained:

$$A_1 = 652 \text{N/m}, \quad A_2 = 521 \text{N/m}, \quad C_1 = 2.7 \cdot 10^{-10} \text{N nm}, \quad C_2 = 8.7 \cdot 10^{-10} \text{N nm}.$$

(26)

Then the following values for stiffness coefficients of macroscopic material can be obtained:

$$A_{1111} = 355 \quad \text{N/m}, \quad C_{1111} = 2 \cdot 10^{-19} \quad \text{N m};$$

$$A_{1122} = 21 \quad \text{N/m}, \quad C_{1122} = -0.4 \cdot 10^{-19} \quad \text{N m};$$

$$A^*_{1212} = 167 \quad \text{N/m}, \quad C_{1212} = 3.7 \cdot 10^{-19} \quad \text{N m};$$

$$A_{3131} = 301 \quad \text{N/m}, \quad C_{1221} = -1.3 \cdot 10^{-19} \quad \text{N m}.$$

(27)

The results for in-plane moduli A_{1111}, A_{1122} give a good correspondence with the results derived from experimental data for bulk graphite [17]. The negative values of C^*_{1122} and C^*_{1221} do not disrupt the positiveness of the potential energy quadratic form that requires the positiveness of the matrixes of the stiffness tensors.

6 Conclusions

The model of the discrete structure of graphene lattice is considered. Four parameters are introduced to model the linear deformation of the covalent bond. Under assumption of long-wave approximation the equivalent continuum is derived. The relations between the elastic moduli of the continuum and the parameters at microlevel are obtained. Thus, if the experiments allow to calculate the macroscopic parameters of interatomic interactions, the elastic moduli can be determined, and vice versa. The available experimental data allow to determine the in-plane components of tensor ${}^4\underline{\underline{A}}$. Component A_{3131} can be determined then for the present model when parameter A_2 is evaluated using the relations with known macroscopic moduli. There is a need to carry out experiments that are able to estimate the moduli of tensor ${}^4\underline{\underline{C}}$. These moduli can be also estimated if parameters of interaction at microlevel are known, for example, from some new experiments or force fields that are already in use. Additional verification is desirable for the results for the components of tensor ${}^4\underline{\underline{C}}$ derived from the parameters of AMBER force field.

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