

Determination of macroscopic characteristics for graphene layer using angle-depending atomic interactions

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Abstract

The purpose of this investigation is to construct a stable model of graphene (monolayer of graphite) using microstructure analysis and to connect parameters of this model with the macro parameters such as Young modulus and Poisson ratio. It is well-known that usage of central interaction can lead to instability of graphene lattice. A model of interaction containing the terms describing the central and angular interaction is considered. The relation between the model parameters and macro characteristics is found. Parameters describing stiffnesses of the bonds are determined using experimental data. It is planned to use the models considered above for description of the deformation processes in graphene layers.

1 Introduction

Graphene is a monolayer of graphite crystal lattice and it attracts a great deal of attention among physicists. It is primarily connected with its unusual electronic and mechanical properties. In the majority of researches graphene is considered to be two-dimensional material with hexagonal lattice and almost ideal location of atoms, which is particularly the reason of great free run's distance of charge carriers (till one micron). As a matter of fact experimentally obtained monolayer of graphene [1] is not absolutely flat: there are some deformations in transverse direction and it the condition of stability [2]. However in this work the fact mentioned above is not taken into consideration and graphene is considered in two-dimensional space.

There are several reasons why mechanical properties of graphene are so interesting. Firstly the carbon nanotubes that are more and more widely applied in medicine and technics are layers of graphene wrapped in one or another way. Secondly the questions concerning the development of composite materials based on graphene

are discussed. Other possible applications of graphene's mechanical properties are widely discussed in the literature. Thus construction of a rational mechanical model of graphene is extremely important.

It is typically to introduce effective interaction potentials to model the interaction between the atoms of crystal lattices. Pair interaction potentials such as Lennard-Jones and Morse potentials are successfully applied for close packed lattices. However when trying to apply these potentials to a model of material with directed crystal bonds one can reveal that it turns out to be unstable. To solve this problem many-body potentials depending on the angles between the bonds are applied. Such potentials for modeling of carbon compounds were proposed by Tersoff and Brenner [3, 4]. Family of MM-potentials and MM3-potential in particular are also efficiently applied. At the same time Brenner and MM3 potentials are the most-used for modeling of carbon nanotubes.

The method of applying many-particle potentials has some difficulties concerned with complex structure of such potentials and large quantity of interaction parameters. That is why another methods are also applied. One of alternatives taking into account the moment contribution in interatomic interaction. In [6, 7] non-central interaction consisting of two components — force described by a force vector and torque described by a torque vector — is used to model lattice of graphite. Torque component is able to carry in additional transversal stiffness in the system which provides with the stability of hexagonal lattice.

There are some other methods of introducing additional stiffness in the system. In [8] a mechanical model of carbon nanotube is proposed. This model is based on applying elastic rods and springs connecting the atoms to provide stability of the system. Another approach introducing rotatory degree of freedom for describing the moment interaction is used in [9] and [10].

Current research is based on theoretical appliance proposed in [11]. Common representation of energy of interaction containing dependence on angles between interatomic bonds is considered. On basis of of this potential and geometry of the lattice macro parameters such as Young modulus, bulk modulus and Poisson ratio are obtained.

Application of developed models in investigation of deformation and oscillation processes that happen in graphene sheets is presumed.

2 Stiffness tensor of two-atomic lattice

Let us consider ideal complex crystal lattice and assume that elementary cell of this lattice contains two atoms. Such kind of lattice is typical for diamond, graphite, hexagonal close-packed (HCC) crystals. Let us assume that each atom interacts only with its closest neighbours and introduce the following notations: α is an index describing the closest neighbours of the selected atom and corresponding bonds, index β describes adjacent atoms and bonds. The energy accounting for one particle can be represented in the following way:

$$W = \frac{1}{V_0} \left(G_1 \sum_{\alpha} \kappa_{\alpha}^2 + G_2 \sum'_{\alpha, \beta} \xi_{\alpha\beta}^2 + G_3 \sum'_{\alpha, \beta} (\kappa_{\alpha} + \kappa_{\beta}) \xi_{\alpha\beta} \right) \quad (1)$$

Here V_0 is volume of the elementary cell, κ_α and κ_β are deformations of the bonds α and β , $\xi_{\alpha\beta}$ is change of the angle between the bonds. Prime next to sum means that summation is carried out by adjacent bonds. It is taken into account that the elementary cell contains two particles and that in the result of summation it is allowed for the same bonds twice. If the interaction is carried out by linear springs with stiffness c and by angular springs with stiffness γ , then

$$G_1 = \frac{1}{2}ca^2, \quad G_2 = \frac{1}{2}\gamma, \quad G_3 = 0, \quad (2)$$

where a is length of the linear spring.

It is well-known that every complex lattice can be represented as a combination of two simple sublattices. Let us assume that deformation of the crystal consists of small homogeneous deformation of its both sublattices. The obtained configuration won't be in equilibrium position but will be tending to this position at the expense of displacement of one sublattice relative to another upon some discrepancy vector $\underline{\zeta}$. Therefore strain energy that on one hand appears to be the quadratic form of strain tensor can be represented as the sum of quadratic and bilinear forms of the strain tensor $\underline{\underline{\varepsilon}}$ and the discrepancy vector $\underline{\zeta}$ on the other hand:

$$W = \frac{1}{2} \underline{\underline{\varepsilon}} \cdot \cdot \underline{\underline{C}} \cdot \cdot \underline{\underline{\varepsilon}} = \frac{1}{2} \underline{\underline{\varepsilon}} \cdot \cdot \underline{\underline{C}}_* \cdot \cdot \underline{\underline{\varepsilon}} + \frac{1}{2} \underline{\zeta} \cdot \underline{\underline{C}} \cdot \underline{\zeta} + \underline{\zeta} \cdot \underline{\underline{C}} \cdot \cdot \underline{\underline{\varepsilon}} \quad (3)$$

Let us assume that the crystal undergoes small strain $\underline{\underline{\varepsilon}}$. The discrepancy vector should provide here with the displacement of the sublattices so that to implement a minimum of the strain energy. This allows to obtain a relation between the discrepancy vector and the strain tensor.

$$\frac{\partial W}{\partial \underline{\zeta}} = 0 \Rightarrow \underline{\underline{C}} \cdot \underline{\zeta} + \underline{\underline{C}}_* \cdot \underline{\underline{\varepsilon}} = 0 \Rightarrow \underline{\zeta} = -\underline{\underline{C}}^{-1} \cdot \underline{\underline{C}}_* \cdot \underline{\underline{\varepsilon}} \quad (4)$$

Using the last relation one can express the stiffness tensor:

$$\underline{\underline{C}} = \underline{\underline{C}}_* - \underline{\underline{C}}_*^T \cdot \underline{\underline{C}}^{-1} \cdot \underline{\underline{C}}_* \quad (5)$$

It is shown in Appendix A that deformations of the bonds can be represented in the following way:

$$\begin{aligned} \kappa_\alpha &= \underline{n}_\alpha \underline{n}_\alpha \cdot \underline{\underline{\varepsilon}} + \underline{n}_\alpha \cdot \underline{\zeta}, & \kappa_{\alpha\beta} &= \underline{n}_\alpha \underline{n}_\beta \cdot \underline{\underline{\varepsilon}} + \frac{1}{2}(\underline{n}_\alpha + \underline{n}_\beta) \cdot \underline{\zeta}, \\ \xi_{\alpha\beta} &= \frac{(\kappa_\alpha + \kappa_\beta) \cos \varphi - 2\kappa_{\alpha\beta}}{\sin \varphi}. \end{aligned} \quad (6)$$

After putting formula (6) in (1) the stiffness tensors from (3) can be expressed:

$$\begin{aligned} \underline{\underline{C}}_* &= \frac{2}{V_0} \left(H_1 \sum_\alpha \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha + H_2 \sum'_{\alpha,\beta} \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\beta \underline{n}_\beta \right) + \\ &+ \frac{2}{V_0} \left(H_3 \sum'_{\alpha,\beta} (\underline{n}_\alpha \underline{n}_\beta \underline{n}_\beta \underline{n}_\alpha + \underline{n}_\alpha \underline{n}_\beta \underline{n}_\alpha \underline{n}_\beta) \right), \\ \underline{\underline{C}} &= \frac{1}{V_0} H_4 \sum_\alpha \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha, & \underline{\underline{C}}_* &= \frac{2}{V_0} H_5 \sum_\alpha \underline{n}_\alpha \underline{n}_\alpha, \end{aligned} \quad (7)$$

where constant coefficients H_k can be calculated using the following formula:

$$\begin{aligned} H_1 &= G_1 - 6M_1G_2 \cot^2 \varphi - 2M_1G_3 \cot \varphi, \\ H_2 &= 2G_2 \cot^2 \varphi + 2G_3 \cot \varphi, \quad H_3 = 2G_2(1 + \cot^2 \varphi), \\ H_4 &= 2G_1 + 4G_2M_1 \frac{\cot \varphi}{\sin \varphi} (1 - \cos \varphi)^2 + 2G_3M_1 \frac{1}{\sin \varphi} (\cos 2\varphi - \cos \varphi), \\ H_5 &= G_1 + 2G_2M_1(1 - \cos \varphi) - 2G_3M_1 \sin \varphi. \end{aligned} \quad (8)$$

While obtaining (7)–(8) formula (50) from Appendix B was used. M_1 is number of bonds adjacent with the selected one, d is dimensionality of space. Formula (7) applying (49) and (52) from Appendix B and taking into consideration symmetry can be represented in the following way:

$$\begin{aligned} {}^2\underline{\underline{C}} &= \frac{2H_5M}{V_0d} \underline{\underline{E}}, \quad {}^3\underline{\underline{C}}^T \cdot {}^3\underline{\underline{C}} = \frac{H_4^2}{V_0^2} \left(\frac{d+1}{d} \sum_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} - \frac{M^2}{d^3} \underline{J}_{\underline{1}} \right), \\ {}^4\underline{\underline{C}}_{**} &= \frac{2}{V_0} \left((H_1 + M_1P(H_2 + 2H_3)) \sum_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} + H_2Q \underline{J}_{\underline{1}} + H_3Q (\underline{J}_{\underline{2}} + \underline{J}_{\underline{3}}) \right); \end{aligned} \quad (9)$$

where

$$Q = \frac{M_1M \sin^2 \varphi}{d(d-1)}, \quad P = \cos^2 \varphi - \frac{\sin^2 \varphi}{d-1}. \quad (10)$$

After putting (9) in (5) the stiffness tensor of the complex lattice can be expressed as

$${}^4\underline{\underline{C}} = \kappa' \sum_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} + \lambda' \underline{J}_{\underline{1}} + \mu' (\underline{J}_{\underline{2}} + \underline{J}_{\underline{3}}), \quad (11)$$

where

$$\begin{aligned} \kappa' &= \frac{2}{V_0} (H_1 + M_1P(H_2 + 2H_3)) - \frac{1}{2MH_5} \frac{H_4^2(d+1)}{V_0}, \\ \lambda' &= \frac{2}{V_0} QH_2 + \frac{MH_4^2}{2d^2H_5V_0}, \quad \mu' = \frac{2}{V_0} QH_3. \end{aligned} \quad (12)$$

Let us consider tensor $\sum_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha}$. In case of orthotropic material with cubic symmetry this tensor can be represented in the following way:

$$\sum_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} = M_{\kappa} \underline{e}_k \underline{e}_k \underline{e}_k \underline{e}_k + M_{\mu} (\underline{J}_{\underline{1}} + \underline{J}_{\underline{2}} + \underline{J}_{\underline{3}}), \quad (13)$$

where \underline{e}_k are unit vectors of cubic sublattice's axes in case of crystals with cubic symmetry or unit vectors of a arbitrary orthonormal basis in case of isotropy of elastic properties; M_{κ} and M_{μ} — dimensionless coefficients defined by formula

$$M_{\kappa} = 2 \frac{1 - \eta_c}{d(d\eta_c + 2)} M, \quad M_{\mu} = \frac{\eta_c}{d(d\eta_c + 2)} M, \quad (14)$$

where η_c — anisotropy parameter of tensor $\sum_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha} \underline{n}_{\alpha}$. It coincides with anisotropy parameter of considered material's stiffness tensor in case of purely force interaction. Anisotropy parameter is usually defined via elastic moduli

$$\eta \stackrel{\text{def}}{=} \frac{2C_{44}}{C_{11} - C_{12}} = \frac{2\mu}{\kappa + 2\mu}. \quad (15)$$

For isotropic material $\eta = 1$. Thus one can rewrite the expression for the stiffness tensor in the following way:

$$\begin{aligned} \underline{\underline{C}} &= \kappa \underline{e}_k \underline{e}_k \underline{e}_k \underline{e}_k + \lambda \underline{J}_{\underline{1}} + \mu (\underline{J}_{\underline{2}} + \underline{J}_{\underline{3}}) \\ \kappa &= \kappa' M_{\kappa}, \quad \lambda = \kappa' M_{\mu} + \lambda', \quad \mu = \kappa' M_{\mu} + \mu', \end{aligned} \quad (16)$$

where κ , λ , μ are generalised Lamé parameters.

In case of isotropy of elastic properties

$$M_{\kappa} = 0, \quad M_{\mu} = \frac{1}{d(d+2)} M \quad (17)$$

and the stiffness tensor takes the canonical form

$$\underline{\underline{C}} = \lambda \underline{J}_{\underline{1}} + \mu (\underline{J}_{\underline{2}} + \underline{J}_{\underline{3}}), \quad (18)$$

where λ and μ are Lamé parameters, which in our case can be expressed in the form

$$\lambda = \frac{M}{d(d+2)} \kappa' + \lambda', \quad \mu = \frac{M}{d(d+2)} \kappa' + \mu', \quad (19)$$

where κ' , λ' , μ' have the form (12). For two-dimensional isotropic material such as sheet of graphene all the stiffness tensor's moduli can be expressed in the following way:

$$\begin{aligned} C_{11} &= \lambda + 2\mu, \quad C_{12} = \lambda, \quad C_{44} = \mu; \quad K = \lambda + \mu, \\ E &= \frac{4\mu(\lambda + \mu)}{\lambda + 2\mu}, \quad \nu = \frac{\lambda}{\lambda + 2\mu}. \end{aligned} \quad (20)$$

3 Determination of elastic characteristics for graphene lattice

Let us consider crystal structure with graphene lattice. An example of such lattice can be found on Figure 1. In case of graphene lattice

$$d = 2, \quad M = 3, \quad M_1 = 2, \quad \varphi = \frac{2\pi}{3}, \quad Q = \frac{9}{4}, \quad P = -\frac{1}{2}, \quad (21)$$

the coefficients H_i can be calculated using the following formula:

$$\begin{aligned} H_1 &= G_1 - 4G_2 + \frac{4\sqrt{3}}{3}G_3, \quad H_2 = \frac{2}{3}(G_2 - \sqrt{3}G_3), \quad H_3 = \frac{8}{3}G_2 \\ H_4 &= 2(G_1 - 6G_2), \quad H_5 = G_1 + 6G_2 - 2\sqrt{3}G_3, \end{aligned} \quad (22)$$

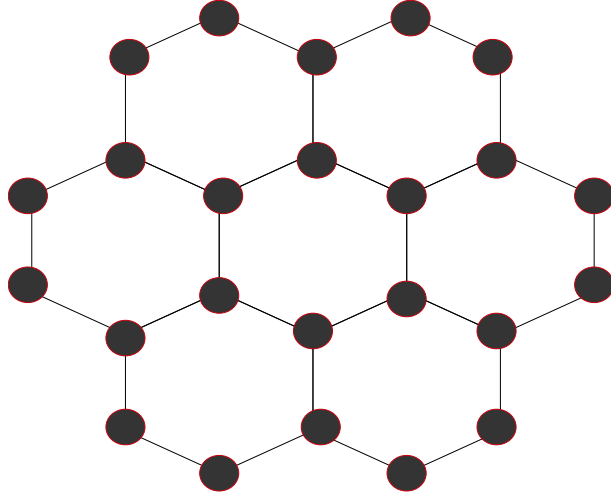


Figure 1: Graphene lattice

and coefficients κ' , λ' and μ' are

$$\kappa' = \frac{2}{V_0} \left(H_1 - H_2 - H_3 - \frac{H_4^2}{4H_5} \right), \quad \lambda' = \frac{3}{4V_0} \left(6H_2 + \frac{H_4^2}{2H_5} \right), \quad (23)$$

$$\mu' = \frac{9}{2V_0} H_3$$

respectively. The volume of the elementary cell is $V_0 = \frac{3\sqrt{3}}{2} a^2$.

Let us assume that the interaction is carried out in correspondence with (35). Here the bulk modulus, Young modulus and the Poisson ratio can be expressed via stiffnesses G_1 and G_2 using (16) and (19):

$$E = \frac{72G_1G_2}{V_0(G_1 + 18G_2)}, \quad \nu = \frac{G_1 - 6G_2}{G_1 + 18G_2}, \quad K = \frac{3G_1}{2V_0}. \quad (24)$$

As one can see the bulk modulus does not depend on the stiffness of the angle interaction G_2 but only on the tension stiffness of the bond as would be expected. After putting (2) in (24) and introducing a notation $c_\gamma = \frac{\gamma}{a^2}$ the following formulae are obtained:

$$E = 8\sqrt{3} \frac{cc_\gamma}{c + 18c_\gamma}, \quad \nu = \frac{c - 6c_\gamma}{c + 18c_\gamma}, \quad K = \frac{\sqrt{3}}{6} c. \quad (25)$$

Let us consider the matrix of the stiffness tensor according to (20)

$$\underline{\underline{C}} \sim \begin{bmatrix} \lambda + 2\mu & \lambda & 0 \\ \lambda & \lambda + 2\mu & 0 \\ 0 & 0 & \mu \end{bmatrix}, \quad (26)$$

where Lamé parameters can be calculated applying formula (19)

$$\lambda = \frac{\sqrt{3}}{6} c \frac{c - 6c_\gamma}{c + 6c_\gamma}, \quad \mu = \frac{2\sqrt{3}cc_\gamma}{c + 6c_\gamma}. \quad (27)$$

The 2D stability criterion can be expressed like this:

$$\begin{cases} \lambda + \mu > 0 \\ \mu > 0 \end{cases} \quad (28)$$

After putting (27) in (28) the criterion can be obtained:

$$\begin{cases} \left[\begin{array}{l} c_\gamma > 0 \\ c_\gamma < -\frac{c}{6} \end{array} \right. \\ c > 0 \end{cases} \quad (29)$$

The same results can be obtained from equations (25) taking into consideration the fact that

$$K > 0, \quad -1 < \nu < 1. \quad (30)$$

According to [12] elastic moduli of this lattice's stiffness tensor are:

$$\frac{C_{11}}{h} = 1060 \text{ GPa}, \quad \frac{C_{12}}{h} = 180 \text{ GPa}, \quad a = 0.142 \text{ nm}, \quad h = 0.34 \text{ nm}, \quad (31)$$

where h is a distance between the graphene planes in graphite crystals. Let us remind that the stiffness coefficients (20) correspond to two-dimensional theory and therefore are measured in N/m whereas obtained experimentally values for graphite correspond to three-dimensional theory and are measured in Pa=N/m². Distance h is a coefficient of proportionality between two-dimensional and three-dimensional elastic moduli (since the volume of three-dimensional graphite crystal's elementary cell is equal to the composition of the volume of two-dimensional graphene's one and the distance h). Putting the experimental data in (20) one can obtain:

$$\begin{aligned} \lambda &= 61.2 \text{ N/m}, & \mu &= 149.6 \text{ N/m}, & K &= 210.8 \text{ N/m} \\ E &= 350.0 \text{ N/m}, & \nu &= 0.17. \end{aligned} \quad (32)$$

Stiffnesses c and c_γ for graphene lattice can be calculated applying (32) and the latter relations:

$$c = 730.2 \text{ N/m}, \quad c_\gamma = 66.9 \text{ N/m}. \quad (33)$$

As one can see from (33) criterion (29) holds true.

4 Conclusion

In this work the general representation for the energy of interatomic interaction including the angles between the atomic bonds was considered. The interaction is carried out by means of linear and angular springs. Representation for complex two-atomic lattice's stiffness tensor is obtained on the basis of proposed model. The elastic characteristics of graphene crystal lattice as well as stiffnesses of torsion and linear springs are determined applying the experimental data. It was shown

that considered model allows to obtain the correct values of the components of the macroscopic stiffness tensors and satisfies the necessary stability conditions.

The performed investigation permitted to build the model of interatomic interaction that can be used for analytical modeling and computer simulations by methods of particle and molecular dynamics to investigate deformation and oscillation processes that happen in graphene sheets.

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Appendixes

A Determination of interatomic bonds' deformations.

Let us consider a deformation of the bonds between the selected particle and its closest neighbours that are indicated with index α . The bond vectors \underline{A}_α in the current configuration can be expressed in the following way:

$$\underline{A}_\alpha = \underline{a}_\alpha + \underline{u}_\alpha - \underline{u} + \underline{a}\underline{\zeta}, \quad (34)$$

where \underline{a}_α is a vector of the bond between the selected particle and the particle α in the initial configuration, \underline{u}_α and \underline{u} – displacements of the particle α and the selected particle respectively, $\underline{\zeta}$ – discrepancy vector (\underline{a} – length of the bond in the initial configuration).

Taking into account long-wave approach one can express

$$\underline{u}_\alpha - \underline{u} = \underline{a}_\alpha \cdot \nabla \underline{u}. \quad (35)$$

Then casting out small terms and applying (34):

$$\underline{A}_\alpha = \underline{a}_\alpha + \underline{a}_\alpha \cdot \nabla \underline{u} + \underline{a}\underline{\zeta}, \quad A_\alpha^2 = a_\alpha^2 + 2\underline{a}_\alpha \underline{a}_\alpha \cdot \underline{\underline{\varepsilon}} + 2\underline{a}_\alpha \cdot \underline{a}\underline{\zeta} \quad (36)$$

The modulus of the bond vector in the current configuration can be expressed in the following way:

$$A_\alpha \simeq a(1 + \underline{n}_\alpha \underline{n}_\alpha \cdot \underline{\underline{\varepsilon}} + \underline{n}_\alpha \cdot \underline{\zeta}). \quad (37)$$

Here the deformation of the bond

$$\kappa_\alpha = \frac{A_\alpha - a_\alpha}{a_\alpha} = \underline{n}_\alpha \underline{n}_\alpha \cdot \underline{\underline{\varepsilon}} + \underline{n}_\alpha \cdot \underline{\zeta}. \quad (38)$$

Let us evaluate the change of the angle φ between the bonds. After introducing the notation $\xi_{\alpha\beta}$ that defines the increment of the angle between the bonds α and β the following equations can be obtained:

$$\cos(\varphi + \xi_{\alpha\beta}) = \frac{\underline{A}_\alpha \cdot \underline{A}_\beta}{A^2} = \cos \varphi - \sin \varphi \xi_{\alpha\beta}. \quad (39)$$

Taking into consideration that $\cos \varphi = (\underline{\mathbf{a}}_\alpha \cdot \underline{\mathbf{a}}_\beta) / \mathbf{a}^2$ and

$$\mathbf{A}_\alpha \cdot \mathbf{A}_\beta = \mathbf{a}_\alpha \cdot \mathbf{a}_\beta + 2\underline{\mathbf{a}}_\alpha \underline{\mathbf{a}}_\beta \cdot \underline{\underline{\boldsymbol{\varepsilon}}} + 2(\underline{\mathbf{a}}_\alpha + \underline{\mathbf{a}}_\beta) \cdot \underline{\mathbf{a}} \underline{\underline{\boldsymbol{\zeta}}}, \quad (40)$$

one can come to the following relation:

$$\cos \varphi - \sin \varphi \xi_{\alpha\beta} = (\cos \varphi + 2\kappa_{\alpha\beta})(1 - \kappa_\alpha)(1 - \kappa_\beta). \quad (41)$$

Here

$$\kappa_{\alpha\beta} = \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\beta \cdot \underline{\underline{\boldsymbol{\varepsilon}}} + \frac{1}{2}(\underline{\mathbf{n}}_\alpha + \underline{\mathbf{n}}_\beta) \cdot \underline{\underline{\boldsymbol{\zeta}}}. \quad (42)$$

And now let us transform (41) and obtain as a result of this transformation

$$\xi_{\alpha\beta} = \frac{(\kappa_\alpha + \kappa_\beta) \cos \varphi - 2\kappa_{\alpha\beta}}{\sin \varphi}. \quad (43)$$

B Some relations for components of the stiffness tensor

Let us consider unit vectors $\underline{\mathbf{n}}_\alpha$ and $\underline{\mathbf{n}}_\beta$ that specify the direction of the adjacent bonds. Then let us represent $\underline{\mathbf{n}}_\beta$ as a sum of two items: one is parallel and another is perpendicular to $\underline{\mathbf{n}}_\alpha$:

$$\underline{\mathbf{n}}_\beta = \underline{\mathbf{n}}_\alpha \cos \varphi + \underline{\mathbf{n}}_a^b \sin \varphi, \quad (44)$$

where $\underline{\mathbf{n}}_a^b$ is a unit vector normal to $\underline{\mathbf{n}}_\alpha$. Let us assume that the following identities hold true owing to the symmetry of the lattice

$$\sum_{\beta(\alpha)} \underline{\mathbf{n}}_a^b = 0, \quad \sum_{\beta(\alpha)} \underline{\mathbf{n}}_a^b \underline{\mathbf{n}}_a^b = \frac{\mathbf{M}_1}{\mathbf{d} - 1} (\underline{\underline{\mathbf{E}}} - \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\alpha), \quad \sum_\alpha \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\alpha = \frac{\mathbf{M}}{\mathbf{d}} \underline{\underline{\mathbf{E}}}, \quad (45)$$

where the summation by $\beta(\alpha)$ means the summation by all the bonds that are adjacent to $\underline{\mathbf{n}}_\alpha$; $\mathbf{d} = 2, 3$ — dimensionality of space; $\underline{\underline{\mathbf{E}}}$ — unit tensor corresponding to the space dimension, \mathbf{M} — the number of closest neighbours for selected atom, \mathbf{M}_1 — the number of the bonds adjacent to the selected one. These identities hold true for the graphite lattice and at least for the following crystal lattices: triangular, simple cubic, square, BCC. Applying formulae (44)–(45) one can obtain

$$\sum_{\beta(\alpha)} \underline{\mathbf{n}}_\beta \underline{\mathbf{n}}_\beta = \mathbf{M}_1 \mathbf{P} \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\alpha + \frac{\mathbf{M}_1}{\mathbf{d} - 1} \underline{\underline{\mathbf{E}}}, \quad \mathbf{P} = \cos^2 \varphi - \frac{\sin^2 \varphi}{\mathbf{d} - 1}. \quad (46)$$

Then the following tensors can be transformed:

$$\begin{aligned} \sum_{\alpha, \beta}' \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\beta \underline{\mathbf{n}}_\beta &= \mathbf{M}_1 \mathbf{P} \sum_\alpha \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\alpha + \mathbf{Q} \underline{\underline{\mathbf{J}}}_1, \\ \sum_{\alpha, \beta}' (\underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\beta \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\beta + \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\beta \underline{\mathbf{n}}_\beta \underline{\mathbf{n}}_\alpha) &= 2\mathbf{M}_1 \mathbf{P} \sum_\alpha \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\alpha \underline{\mathbf{n}}_\alpha + \mathbf{Q} (\underline{\underline{\mathbf{J}}}_2 + \underline{\underline{\mathbf{J}}}_3), \end{aligned} \quad (47)$$

where $\underline{J}_{\underline{k}}$ — isotropic tensors of forth rank

$$\underline{J}_{\underline{1}} = \underline{e}_k \underline{e}_k \underline{e}_n \underline{e}_n = \underline{\underline{E}} \underline{\underline{E}}, \quad \underline{J}_{\underline{2}} = \underline{e}_k \underline{e}_n \underline{e}_n \underline{e}_k, \quad \underline{J}_{\underline{3}} = \underline{e}_k \underline{e}_n \underline{e}_k \underline{e}_n, \quad (48)$$

where \underline{e}_k are vectors of some orthonormal basis. Here and further the summation by the recurring Latin index is applied. The following notation was introduced:

$$Q = \frac{M_1 M \sin^2 \varphi}{d(d-1)}. \quad (49)$$

The following identities are useful for derivation of the formula for the stiffness tensor:

$$\begin{aligned} \sum_{\alpha, \beta}' \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha &= M_1 \sum_{\alpha} \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha, & \sum_{\alpha, \beta}' \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha &= M_1 \sum_{\alpha} \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha, \\ \sum_{\alpha, \beta}' \underline{n}_\alpha \underline{n}_\alpha &= M_1 \sum_{\alpha} \underline{n}_\alpha \underline{n}_\alpha, \\ \sum_{\alpha, \beta}' \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\beta &= M_1 \cos \varphi \sum_{\alpha} \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha, \\ \sum_{\alpha, \beta}' \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\beta &= M_1 \cos \varphi \sum_{\alpha} \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha, & \sum_{\alpha, \beta}' \underline{n}_\alpha \underline{n}_\beta &= M_1 \cos \varphi \sum_{\alpha} \underline{n}_\alpha \underline{n}_\alpha. \end{aligned} \quad (50)$$

It is not difficult to obtain the formula

$$\underline{a}_m \cdot \underline{a}_n = \begin{cases} a^2, & \mu = \nu; \\ -a^2/d, & \mu \neq \nu \end{cases} \iff \underline{a}_m \cdot \underline{a}_n = \frac{1}{d} a^2 \left((d+1) \delta_{mn} - 1 \right) \quad (51)$$

if one takes into account the symmetry of the lattice. Here δ_{mn} — Kronecker symbol. Applying formula (51) allows to express the following composition:

$$\sum_{\alpha} \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha \cdot \sum_{\alpha} \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha = \frac{d+1}{d} \sum_{\alpha} \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha \underline{n}_\alpha - \frac{1}{d} \left(\sum_{\alpha} \underline{n}_\alpha \underline{n}_\alpha \right) \left(\sum_{\alpha} \underline{n}_\alpha \underline{n}_\alpha \right). \quad (52)$$

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