

# DETERMINATION OF MECHANICAL PROPERTIES OF NANOSTRUCTURES WITH COMPLEX CRYSTAL LATTICE USING MOMENT INTERACTION AT MICROSCALE

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**Abstract.** The paper considers a discrete nano-crystalline model with complex crystal lattices. There are non close-packed lattices, typical for some metals and for solids with covalent bonds, for example, diamond, graphite. Traditionally to describe this kind of lattices one used many-particle-interaction potentials. The alternative approach considers rotational degree of freedom and allows the moment contribution in interatomic interaction. The particles interact, using forces and moments. In this paper the characteristics of interatomic bonds are determined for crystals with diamond structure (carbon, silicon, and germanium). It is shown that relation of bending stiffness of carbon covalent bonds to longitudinal one is between 0.49 – 0.72 (in diamond crystals). Hence, the bending stiffness is comparable with longitudinal, and it should be taken into account on calculation for covalent crystals. For crystals of silicon and germanium, this relation is equal 0.34. The strength of covalent bonds decreases with the rise of interatomic distance in sequence C-Si-Ge.

## 1. COMPLEX CRYSTAL LATTICES

A simple lattice is a lattice with equivalent nodes. For the simple lattice the translation along the vector connecting any two nodes is an identical transformation (for example, a simple cubic lattice). A complex crystal lattice is a lattice which does not possess this property (for example, graphite, diamond, NaCl lattice). A discrete mechanical model for the complex crystal lattice was developed in [1]. The particles in the lattice have translational and rotational degrees of freedom. The particles interact by means of forces and moments. Macroscopic characteristics of crystals depend on longitudinal stiffness of interatomic bonds as well as on transversal stiffness.

The equations for macroscopic stiffness tensor can be expressed in terms of interatomic bonds stiffness tensor and vectors  $\underline{a}_{\alpha\beta}^{\gamma}$ . These vectors

determine lattice geometry: here  $\alpha$  is the cell number,  $\underline{a}_{\alpha\beta}^{\gamma}$  is the vector connecting particle  $\gamma$  of a given cell with particle  $\beta$  from cell  $\alpha$  there are two particles in each cell,  $\beta$  and  $\gamma$ .

The macroscopic power stiffness tensor is given by:

$$\begin{aligned} \underline{\underline{A}}^4 &= \underline{\underline{A}}^4 - \underline{\underline{A}}^4, \quad \underline{\underline{A}}^4 = \frac{1}{2V} \sum_{\alpha\beta\gamma} \underline{a}_{\alpha\beta}^{\gamma} \underline{\underline{A}}_{\alpha\beta}^{\gamma} \underline{a}_{\alpha\beta}^{\gamma}, \\ \underline{\underline{A}}^4 &= 2 \left( \underline{\underline{A}}^3 \right) \cdot \left( \underline{\underline{A}} \right)^{-T} \cdot \left( \underline{\underline{A}}^3 \right)^T, \\ \underline{\underline{A}}^3 &= \frac{1}{2V} \sum_{\alpha\beta\gamma} \underline{a}_{\alpha\beta}^{\gamma} \underline{\underline{A}}_{\alpha\beta}^{\gamma}. \end{aligned} \tag{1}$$

The component  $\underline{\underline{A}}^4$  is the stiffness tensor under uniform deformation,  $\underline{\underline{A}}^4$  is a correction component describing shift between two sublattices,  $V$  is

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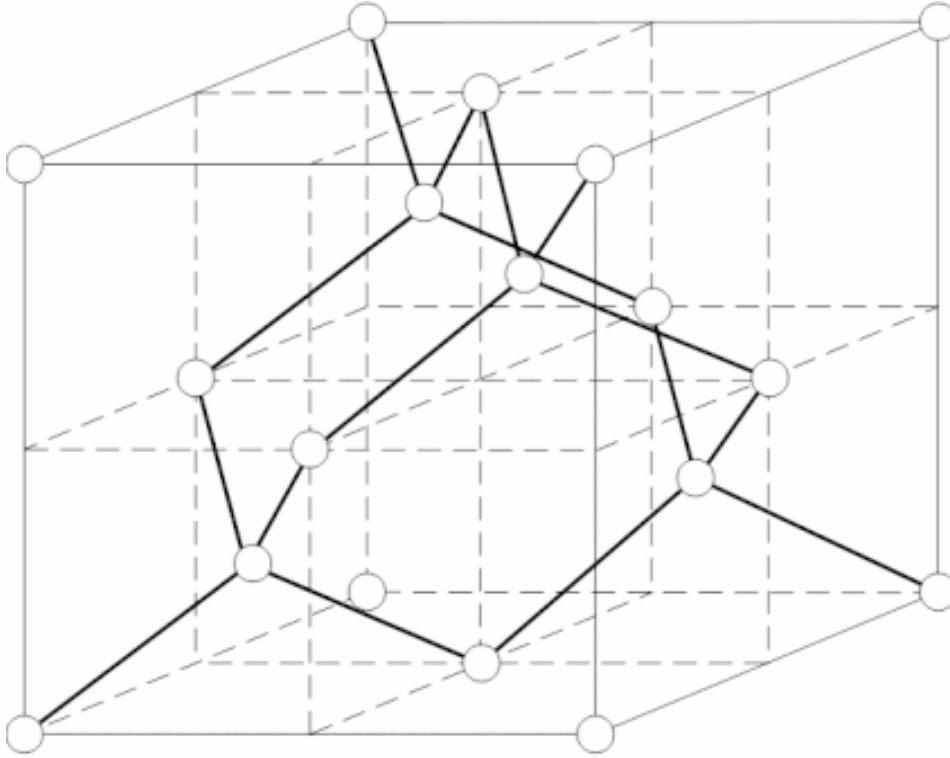


Fig. 1. Diamond lattice.

the unit cell volume. The stiffness tensors of interatomic bonds, we can represent as:

$$\begin{aligned} \underline{\underline{A}}_{\alpha\beta}^{\gamma} &= A_{\alpha\beta}^{\gamma} \underline{\underline{a}}_{\alpha\beta}^{\gamma} \underline{\underline{a}}_{\alpha\beta}^{\gamma} + D_{\alpha\beta}^{\gamma} \underline{\underline{d}}_{\alpha\beta}^{\gamma} \underline{\underline{d}}_{\alpha\beta}^{\gamma}, \\ \underline{\underline{a}}_{\alpha\beta}^{\gamma} \underline{\underline{a}}_{\alpha\beta}^{\gamma} + \underline{\underline{d}}_{\alpha\beta}^{\gamma} \underline{\underline{d}}_{\alpha\beta}^{\gamma} &= (\underline{\underline{a}}_{\alpha\beta}^{\gamma})^2 \underline{\underline{E}}. \end{aligned} \quad (2)$$

The coefficients  $A_{\alpha\beta}^{\gamma}$  in (2) describe longitudinal stiffness of an interatomic bond, coefficients  $D_{\alpha\beta}^{\gamma}$  – transversal stiffness of interatomic bond. In a non-deformed state, the distance between neighboring atoms is  $a$ . Each atom interacts only with the nearest neighbor atoms. In that case all nonzero stiffness coefficients are equal and we can write:

$$A_{\alpha\beta}^{\gamma} = A_{\alpha} = A \quad D_{\alpha\beta}^{\gamma} = D_{\alpha} = D \quad \underline{\underline{a}}_{\alpha\beta}^{\gamma} = \underline{\underline{a}}_{\alpha}. \quad (3)$$

## 2. ELASTIC PROPERTIES OF NANOCRYSTAL WITH 3D DIAMOND LATTICE

Now we consider a three-dimensional crystal with a diamond lattice (Fig. 1), lattice orientation is  $\{100\}$ . Let  $\underline{i}$ ,  $\underline{j}$  and  $\underline{k}$  be the unit vectors of lattice principal directions. Then vectors  $\underline{\underline{a}}_{\alpha\beta}^{\gamma}$  will be equal:

$$\begin{aligned} \underline{\underline{a}}_1 &= \frac{a}{\sqrt{3}}(-\underline{i} + \underline{j} + \underline{k}), \quad \underline{\underline{a}}_2 = \frac{a}{\sqrt{3}}(\underline{i} + \underline{j} - \underline{k}), \\ \underline{\underline{a}}_3 &= \frac{a}{\sqrt{3}}(\underline{i} - \underline{j} + \underline{k}), \quad \underline{\underline{a}}_4 = \frac{a}{\sqrt{3}}(-\underline{i} - \underline{j} - \underline{k}). \end{aligned} \quad (4)$$

Substituting (4) in formula (1), we obtain the expressions for stiffness coefficients of diamond:

$$\begin{aligned} A_{1111} &= A_{2222} = A_{3333} = \frac{4a^4}{9V}(A + 2D), \\ A_{1122} &= A_{1133} = A_{2211} = A_{2233} = A_{3311} = \\ A_{3322} &= \frac{4a^4}{9V}(A - D). \end{aligned} \quad (5)$$

For elasticity modulus (5), the expression for the correction component  ${}^4\underline{\underline{A}}$  is equal zero. This allows simplify the formulae. As is known from the classical theory of elasticity, cubic crystals have three independent elastic constants. The coefficients  $A_{1111}$ ,  $A_{1122}$  and shear modulus can be chosen as these constants. The shear modulus in the moment theory is determined by expression (6)

**Table 1.** Experimental data for diamond elastic constants.

No	$K$ , GPa	$C_{11}$ , GPa	$C_{12}$ , GPa	$C_{44}$ , GPa	$E$ , GPa	Ref
1	542	1076	275	519	964	[2]
2	442	1079	124	578	1053	[3]

The following notations are used:  $A_{1111} = C_{11}$   $A_{1122} = C_{12}$   $G = C_{44}$ .

**Table 2.** Calculated elastic constants for diamond.

No	$Aa^2$ , N/m	$Da^2$ , N/m	$D/A$	$C_{44}$ , GPa
1	578.0	285	0.49	605.2
2	471.6	340	0.72	587.3

Interatomic distance in diamond crystals is  $a = 0.154$  nm.

$$G = \frac{1}{2}(A_{1212} + A_{1221}). \quad (6)$$

Using formulae (1) and (4) we obtain

$$\begin{aligned} A_{1212} &= A_{1212}^* + A_{1212}^i = \frac{12a^4}{9V} \frac{D(A-D)}{A+2D}, \\ A_{1221} &= A_{1221}^* + A_{1221}^i = \frac{12a^4}{9V} \frac{D(2A+D)}{A+2D}. \end{aligned} \quad (7)$$

Returning to (6), we obtain for the shear modulus

$$G = \frac{18a^4}{9V} \frac{AD}{A+2D}. \quad (8)$$

The unit cell volume can be found, using (4), as

$$\begin{aligned} V &= \underline{b}_1 \cdot (\underline{b}_2 \times \underline{b}_3), \quad \underline{b}_\alpha = \underline{a}_\alpha - \underline{a}_4, \\ V &= \frac{16\sqrt{3}}{9} a^3, \quad \alpha = 1,2,3. \end{aligned} \quad (9)$$

Substituting (9) in (5) and (6), we finally obtain the formulae for the three independent elastic constants. They are expressed through stiffness of an interatomic bond and interatomic distance  $a$ :

$$\begin{aligned} A_{1111} &= \frac{\sqrt{3}a}{12}(A+2D); \quad A_{1122} = \frac{\sqrt{3}a}{12}(A-D); \\ G &= \frac{3\sqrt{3}a}{8} \frac{AD}{A+2D}. \end{aligned} \quad (10)$$

Expression (11) shows the connection between the coefficients of the stiffness tensor and Young modules:

$$\begin{aligned} E_1 &= \frac{D}{A_{2222}A_{3333} - A_{2233}A_{3322}}, \\ E_2 &= \frac{D}{A_{1111}A_{3333} - A_{1133}A_{3311}}, \\ E_3 &= \frac{D}{A_{1111}A_{2222} - A_{1122}A_{2211}}, \end{aligned} \quad (11)$$

$$\begin{aligned} D &= A_{1111}A_{2222}A_{3333} + A_{1122}A_{2233}A_{3311} + \\ &A_{1133}A_{2211}A_{3322} - A_{1122}A_{2222}A_{3311} - \\ &A_{1111}A_{2233}A_{3322} - A_{3333}A_{2211}A_{1122}. \end{aligned}$$

The bulk modulus for tensor  $\underline{\underline{A}}$  can be determined by formula (12):

$$K = \frac{1}{d^2} \underline{\underline{E}} \cdot \underline{\underline{A}} \cdot \underline{\underline{E}}. \quad (12)$$

In our case it has the form:

$$K = \frac{4}{9V} Aa^4. \quad (13)$$

As was expected, the bulk modulus depends on the coefficient  $A$  only, which characterizes longitudinal stiffness of an interatomic bond, and does not depend on the coefficient  $D$ , which characterizes transversal stiffness of an interatomic bond.

As is known from the classical theory of elasticity (momentless), there are only three indepen-

**Table 3.** Experimental data for silicon elastic constants.

No	$K$ , GPa	$C_{11}$ , GPa	$C_{12}$ , GPa	$C_{44}$ , GPa	$E$ , GPa	Ref
1	98	166	64	80	130	[4]

**Table 4.** Calculated elastic constants for silicon.

$Aa^2$ , N/m	$Da^2$ , N/m	$D/A$	$C_{44}$ , GPa
159.6	55	0.34	90

Interatomic distance in silicon crystals is  $a = 0.235$  nm.

**Table 5.** Experimental data for germanium elastic constants.

$K$ , GPa	$C_{11}$ , GPa	$C_{12}$ , GPa	$C_{44}$ , GPa	$E$ , GPa	Ref
71	126	44	67	103	[4]

**Table 6.** Calculated elastic constants for germanium.

$Aa^2$ , N/m	$Da^2$ , N/m	$D/A$	$C_{44}$ , GPa
121	46	0.38	70

Interatomic distance in germanium crystals is  $a = 0.245$  nm.

**Table 7.** Comparative table of calculated transversal and longitudinal stiffness for elements with diamond structure.

	$Aa^2$ , N/m	$Da^2$ , N/m	$D/A$	$a$ , nm
C	578	285	0.49	0.154
C	472	340	0.72	
Si	160	55	0.34	0.235
Ge	121	46	0.38	0.245

dent elastic constants, for example (10). If the values of these elastic constants are known for some material, then expressions (10) allow find microscopic characteristics of interatomic bonds, coefficients  $A$  and  $D$ . Thus, momentless macroscopic characteristics of a material allow find power characteristic interatomic bond  $A$  and coefficient  $D$ . The coefficient  $D$  characterizes the transversal stiffness interatomic bond. It should be noted that this coefficient presents only in the models which take into account a moment interaction on the interatomic level.

Experimental data for diamond elastic constants [2,3] are shown in Table 1, bulk modules  $K$  and young modules  $E$  are calculated from (11,13). As one can see, these data are not the same for different experimental methods.

Using experimental data [2] for  $C_{11}$  and  $C_{12}$  and formulas (10), we obtain the value of stiffness of interatomic bonds in diamond crystals:

$$Aa^2 = 578 \text{ N/m} \quad Da^2 = 285 \text{ N/m}. \quad (14)$$

Hence, the ratio *transversal stiffness / longitudinal stiffness* in a diamond crystal is  $D/A = 0.49$ .

Using experimental data [3] for and  $C_{11}$  and formulae (10), we obtain the value of stiffness of interatomic bonds in diamond crystals:

$$Aa^2 = 472 \text{ N/m}, \quad Da^2 = 340 \text{ N/m}. \quad (15)$$

Hence, the ratio *transversal stiffness / longitudinal stiffness* in a diamond crystal is  $D/A = 0.72$ . It means that in both cases the transversal stiffness is of the same order as longitudinal one, and thus has to be taken into account when investigating covalent crystals.

Using coefficients (14), (15) and formulae (10), (11) we can determine the value of elastic constants (Table 2).

As one can see from Tables 1 and 2, the calculated data are nearer to the experimental ones in the second case. The maximum deviation does not exceed 1.6% in the second case, whereas in the first case it is equal to 16.6%.

Analogously we consider silicon. Silicon has a diamond structure too. The experimental data for silicon elastic constants [4] are shown in Table 3.

Using experimental data for and  $C_{11}$ , and formulae (10), we obtain the value of stiffness of interatomic bonds in silicon crystals:

$$Aa^2 = 160 \text{ N/m}, \quad Da^2 = 55 \text{ N/m}. \quad (16)$$

so that  $D/A = 0.344$ .

The substitution of coefficients (16) into formulae (10), (11) gives the value of elastic constants (Table 4).

In this case the maximum deviation from the experimental data is 13%.

We performed similar calculation for germanium, since it has a diamond structure too. Experimental data for germanium are shown in Table 5.

The value of stiffness of interatomic bonds in germanium crystals:

$$Aa^2 = 121 \text{ N/m}, \quad Da^2 = 46 \text{ N/m}. \quad (17)$$

with  $D/A = 0.38$ . From (17) we calculated the value of elastic constants for germanium (Table 6).

In this case the maximum deviation from experimental data is 4.5%. Thus, from the above results it is seen that the method considered gives a good coincidence with the experimental data. The maximum deviation is 16.6%. However, it is necessary to take into account the spread of experimental values.

Table 7 makes a comparison of the calculated transversal and longitudinal stiffness for elements with diamond structure (carbon, silicon, germanium). From it follows that in the C-Si-Ge series the stiffness of covalent bonds decreases with the increase of an interatomic distance

### 3. CONCLUSIONS

For crystals with diamond structure, such as carbon, silicon, germanium, the equations for macroscopic tensors of stiffness are obtained. They depend on tensors of stiffness of interatomic bonds and vectors, which define the geometry of the lattice. The characteristics of the interatomic bonds are also defined. It is shown that the ratio *transversal stiffness / longitudinal stiffness* of carbon's covalent bond is between 0.72 and 0.49. It means that the transversal stiffness is of the same order as longitudinal one, and thus has to be taken into account when investigating covalent crystals. In the C-Si-Ge series, the stiffness of covalent bonds decreases with the increase of an interatomic distance.

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