FORCE AND ELASTIC CONSTANTS OF METALS AND ALLOYS

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Abstract. A review of theoretical and experimental investigations of elastic constants of metals and alloys is done. It is considered method of calculations of force and elastic constants of metals by using model potential of Heine-Abarenkov-Animalu within pseudopotential theory. Thus, it is paid especially attention to methods of calculations of elastic constants, in which established a relation between force constants and elastic constants according a long wave approximation. Shown, that pseudopotential method allows to calculate force and elastic constants of metals and alloys.

Keywords: metals, alloys, elastic constants, dynamical matrix, force constants, pseudopotential method

PACS 61.10.Eq

Bibliography – 65 references

Received 15.05.2015

RENSIT, 2015, 7(1):68-86

DOI: 10.17725/rensit.2015.07.068

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1. INTRODUCTION

Force constants of atomic interactions in solids are important both in practical and fundamental terms, as elasticity, hardness, thermal capacity of bodies and dynamics of a crystal lattice depend on them [1]. Values of force constants contain information on nature and long-range interaction of interatomic forces, characterize a potential of atomic interaction. These constants depend on a lattice configuration, so they are important in calculations of stability of crystalline orders and entropy contribution to internal energy of a crystal lattice. In calculations of a lattice dynamics and force constants for atomic interaction, the Born-Karman force constants and also radial and tangential force constants are most widely applied.

The pseudopotential theory allows to calculate force constants of atomic interaction, by means of which we can receive formulas in long-wave approximation for calculation of elastic constants for metal elements of a dynamic matrix and apply them in calculations of elastic constants in comparison with experimental data.

In this work we set a goal to summarize results of researches, conducted in this aspect, and to compare with results, received by other methods of calculation for elastic constants, among which are the method of homogeneous deformations and density functional theory.

2. FORCE CONSTANTS IN THE BORN-VON KARMAN AND DE LANE MODELS

Force constants Φ_{ij}^s in the Born-Karman model express force that acts in the i -direction to an atom, which locates in the reference point, when the closest j -atom moves to the length unit in the j -direction ($i, j = x, y, z$). Therefore, an array of force constants Φ_{ij}^s is represented in the form [2]:

$$\begin{vmatrix} \alpha_1^s & \beta_3^s & \beta_2^s \\ \beta_3^s & \alpha_2^s & \beta_1^s \\ \beta_2^s & \beta_1^s & \alpha_3^s \end{vmatrix}. \quad (1)$$

In the case of axially symmetric forces, a set of force constants for any neighboring atom depends only on two independent parameters that can be selected as radial Φ_r^s and tangential Φ_t^s force constants. These constants have the following form [3]:

$$\Phi_r^s = \left(\frac{\partial^2 V}{\partial r^2} \right)_{r=r^s}, \quad \Phi_t^s = \left(\frac{1}{r} \frac{\partial V}{\partial r} \right)_{r=r^s}. \quad (2)$$

Here V is an atomic interaction potential, r^s is an equilibrium position of the s -neighboring atom with respect to the reference point

$$\mathbf{r}^s = \frac{1}{2} a (h_1^s \hat{\mathbf{i}} + h_2^s \hat{\mathbf{j}} + h_3^s \hat{\mathbf{k}}), \quad (3)$$

where a – a lattice parameter, h_1^s, h_2^s, h_3^s – integers, $\hat{\mathbf{i}}, \hat{\mathbf{j}}, \hat{\mathbf{k}}$ – basis vectors in directions of coordinate axes. Force constants Φ_{ij}^s can be written as:

$$\Phi_{ij}^s = \frac{a^2 h_i^s h_j^s}{4(r^s)^2} (\Phi_r^s - \Phi_t^s) + \delta_{ij} \Phi_t^s, \quad (4)$$

where δ_{ij} is a Kronecker symbol. There is also a symbol $K_{ij} = \Phi_{ij}^s$. A number of independent force constants K_{ij} in a particular coordination sphere, as can be seen from equation (4), depend on coordinates h_1^s, h_2^s, h_3^s of atoms in a given sphere. For example, for FCC structure in a first sphere of atomic coordinates [110], three

independent force constants are determined due to this reason:

$$\begin{vmatrix} K_{xx} & K_{xy} & 0 \\ K_{xy} & K_{yy} & 0 \\ 0 & 0 & K_{zz} \end{vmatrix}.$$

In the second sphere of atomic coordinates [200] only two independent constants are determined:

$$\begin{vmatrix} K_{xx} & 0 & 0 \\ 0 & K_{yy} & 0 \\ 0 & 0 & K_{zz} \end{vmatrix}.$$

In the third sphere of atomic coordinates [211] – four independent constants:

$$\begin{vmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{xy} & K_{yy} & K_{yz} \\ K_{xz} & K_{yz} & K_{zz} \end{vmatrix}.$$

Thus, it is possible to determine the force constants of the Born-Karman in any sphere, and, thus, the maximum number of independent constants is six.

The Hooke's force constants of radial and tangential forces of atomic interaction are considered in the De Launays model [4]. To calculate an elastic force that acts between the atom O , located at the reference point, and its neighbor with n index, it is necessary to consider their relative displacement. We will take a unit vector $\mathbf{e}_n$, which is directed along a line, connecting equilibrium positions of these atoms (**Fig. 1**). We will designate as $\mathbf{a}_n$ the Hooke's constant for interaction force of these atoms, which can be called a radial force constant. Vectors $\mathbf{s}_0$ and $\mathbf{s}_n$ on Fig. 1 respectively designate displacements of O and n atoms from their equilibrium positions. If

Fig. 1. Displacements of the atoms with indices 0 and n out of equilibrium.

$s_0 - s_n = 0$, the distance between these atoms will not change. In general case the distance between atoms changes and a component of this change along $\mathbf{e}_n$ will be $\mathbf{e}_n \cdot (s_0 - s_n)$. Therefore, a radial restoring force, acting on an atom O from an atom n , is equal to $F_n = -a_n [\mathbf{e}_n \cdot (s_0 - s_n)] \cdot \mathbf{e}_n$. If we designate the direction cosines of $\mathbf{e}_n$ as λ_n, μ_n, ν_n , the force components F_n will be equal

$$\begin{aligned} X_n &= -a_n \lambda_n [\lambda_n (u_0 - u_n) + \mu_n (v_0 - v_n) + \nu_n (w_0 - w_n)]; \\ Y_n &= -a_n \mu_n [\lambda_n (u_0 - u_n) + \mu_n (v_0 - v_n) + \nu_n (w_0 - w_n)]; \\ Z_n &= -a_n \nu_n [\lambda_n (u_0 - u_n) + \mu_n (v_0 - v_n) + \nu_n (w_0 - w_n)]; \end{aligned} \quad (5)$$

where u_0, v_0, w_0 – components of the vector s_0 ; u_n, v_n, w_n are components of the vector s_n . Components X_n, Y_n, Z_n of a radial elastic force, acting on the O atom from the atom with n index, are included in the equation of motion along the coordinate axes:

$$M\ddot{u}_0 = \sum_n X_n; M\ddot{v}_0 = \sum_n Y_n; M\ddot{w}_0 = \sum_n Z_n, \quad (6)$$

where the sum is taken over all n neighboring atoms.

For calculation of tangential forces, we should express the displacement components of the vectors $\mathbf{s}_0$ and $\mathbf{s}_n$, which are perpendicular to a line, connecting the equilibrium positions of atoms with indexes O and n . First, we consider the vector $\mathbf{s}_0$. A component of this vector, perpendicular to a connecting line of equilibrium positions of the considered atoms, given as $\mathbf{e}_n \times \mathbf{s}_0$. But this vector product is perpendicular to a plane of multiplied vectors. If we in addition multiply vectorially $(\mathbf{e}_n \times \mathbf{s}_0) \times \mathbf{e}_n$, we will receive a desired direction and the value $|\mathbf{e}_n \times \mathbf{s}_0|$ will remain. In general, the result of displacement of the considered atoms will be $[\mathbf{e}_n \times (\mathbf{s}_0 - \mathbf{s}_n)] \times \mathbf{e}_n$ and elastic force will be expressed as

$$\mathbf{F}_n = -\beta_n [\mathbf{e}_n \times (\mathbf{s}_0 - \mathbf{s}_n)] \times \mathbf{e}_n, \quad (7)$$

where β_n is tangential force constant between atoms with indexes O and n .

Applying a formula $A \times (B \times C) = B(A \cdot C) - C(A \cdot B)$, we will receive

$$\mathbf{F}_n = -\beta_n (\mathbf{s}_0 - \mathbf{s}_n) + \beta_n [\mathbf{e}_n (\mathbf{s}_0 - \mathbf{s}_n) \cdot \mathbf{e}_n],$$

which in the form of components can be represented as:

$$\begin{aligned} X_n &= -\beta_n \{u_0 - u_n - \\ &\quad - \lambda_n [\lambda_n (u_0 - u_n) + \mu_n (v_0 - v_n) + \nu_n (w_0 - w_n)]\}; \\ Y_n &= -\beta_n \{v_0 - v_n - \\ &\quad - \mu_n [\lambda_n (u_0 - u_n) + \mu_n (v_0 - v_n) + \nu_n (w_0 - w_n)]\}; \\ Z_n &= -\beta_n \{w_0 - w_n - \\ &\quad - \nu_n [\lambda_n (u_0 - u_n) + \mu_n (v_0 - v_n) + \nu_n (w_0 - w_n)]\}; \end{aligned} \quad (8)$$

These components of restoring force can be substituted in the equation of motion (6).

Thus, combining radial and tangential components of restoring force, we will receive:

$$\begin{aligned} X_n &= -\beta_n (u_0 - u_n) - \\ &\quad - (\alpha_n - \beta_n) \lambda_n [\lambda_n (u_0 - u_n) + \mu_n (v_0 - v_n) + \nu_n (w_0 - w_n)]; \\ Y_n &= -\beta_n (v_0 - v_n) - \\ &\quad - (\alpha_n - \beta_n) \mu_n [\lambda_n (u_0 - u_n) + \mu_n (v_0 - v_n) + \nu_n (w_0 - w_n)]; \\ Z_n &= -\beta_n (w_0 - w_n) - \\ &\quad - (\alpha_n - \beta_n) \nu_n [\lambda_n (u_0 - u_n) + \mu_n (v_0 - v_n) + \nu_n (w_0 - w_n)]; \end{aligned} \quad (9)$$

For calculation of the O atom's movement, it is necessary to substitute the formulas (9) into the equation (6), to summarize on index n and solutions are sought in the form:

$$\begin{aligned} u_0 &= A_1 \exp(2\pi i \nu t); \\ v_0 &= A_2 \exp(2\pi i \nu t); \\ w_0 &= A_3 \exp(2\pi i \nu t); \\ u_n &= A_1 \exp(2\pi i \nu t - \mathbf{k} \cdot \mathbf{r}_n); \\ v_n &= A_2 \exp(2\pi i \nu t - \mathbf{k} \cdot \mathbf{r}_n); \\ w_n &= A_3 \exp(2\pi i \nu t - \mathbf{k} \cdot \mathbf{r}_n); \end{aligned}$$

where $\mathbf{k}$ is a wave vector, $\mathbf{r}_n$ is a radius vector of an atom with n index. Thus, a secular equation for calculation of normal vibrational modes of atoms is done in the [4] for a two-dimensional lattice, taking into account a radial interaction with the first two neighboring atoms, and then the same was carried out for *BCC* and *FCC* lattices.

In the above definition (2), radial and tangential force constants are designated by Φ_r^s and Φ_t^s , and in the De Launays model we designated them as α_n and β_n ($n = s$).

3. BORN-BEGBIE MODEL

In the Born-Begbie model [5], the dynamic matrix elements of body-centered cubic structure are expressed through elastic constants c_{11} , c_{12} and c_{44} by means of expressions

$$\begin{aligned} D_{11} &= 2ac_{44} \left[1 - \cos \frac{aq_1}{2} \cos \frac{aq_2}{2} \cos \frac{aq_3}{2} \right] + \\ &+ a(c_{11} - c_{44})[1 - \cos(aq_1)], \\ D_{11} &= D_{22} = D_{33}, \end{aligned} \quad (10)$$

$$\begin{aligned} D_{12} &= 2a(c_{12} + c_{44}) \sin \frac{aq_1}{2} \sin \frac{aq_2}{2} \sin \frac{aq_3}{2}, \\ D_{12} &= D_{21} = D_{13} = D_{31} = D_{23} = D_{32}. \end{aligned}$$

The same kind of thing for face-centered cubic structure:

$$\begin{aligned} D_{11} &= ac_{11} \left[2 - \cos \frac{aq_1}{2} (\cos \frac{aq_2}{2} + \cos \frac{aq_3}{2}) \right] + \\ &+ a(2c_{44} - c_{11})[1 - \cos \frac{aq_2}{2} \cos \frac{aq_3}{2}], \\ D_{11} &= D_{22} = D_{33}, \end{aligned} \quad (11)$$

$$\begin{aligned} D_{12} &= a(c_{12} + c_{44}) \sin \frac{aq_1}{2} \sin \frac{aq_2}{2}, \\ D_{12} &= D_{21} = D_{13} = D_{31} = D_{23} = D_{32}. \end{aligned}$$

In these expressions, a is lattice crystal parameter. The frequency of long-wavelength phonons (sound waves in the crystal) are found using the secular equation

$$|D_{ij} - \rho\omega^2 I| = 0, \quad (12)$$

where ρ is the density of the crystal, ω is cyclic frequency of the phonons, I is the identity matrix. Wave velocities in the crystal can be expressed from the dispersion of sound waves $\omega(q)$ through elastic constants C_{11} , C_{12} , C_{44} .

4. CALCULATION METHOD OF LATTICE DYNAMICS IN THE BORN-VON KARMAN MODEL

Within the Born-Karman model, restoring force between two atoms depends on linearly their relative shift. The motion equation of ℓ th-atom (atom ℓ th-primitive cell) has the form for a particular vibrational mode in the particular direction of symmetry [6]:

$$M\ddot{u}_{\alpha\ell} = -\sum_{\ell'} \Phi_{\alpha\alpha}(\ell, \ell') u_{\alpha\ell'}, \quad (13)$$

where $u_{\alpha\ell}$ is the shift of atom ℓ along particular direction α (polarization), M is the atomic mass, $\Phi_{\alpha\alpha}(\ell, \ell')$ is the restoring force exerted on atom ℓ in the direction α when the atom ℓ' is shifted unit in the direction α (here is specified $\Phi_{ij}^s = \Phi_{\alpha\alpha}(\ell, \ell')$, $\alpha = i, j$ и $s = \ell - \ell'$). The summation contains the term $\ell = \ell'$ and $\sum_{\ell'} \Phi_{\alpha\alpha}(\ell, \ell')_{\alpha\alpha} = 0$ as in the process of uniform shift, the crystal has to be stable. The solution of the equation (1) has a form of the traveling wave:

$$u_{\alpha\ell'} = U_{\alpha} \exp(i\mathbf{q} \cdot \mathbf{R}_{\ell'}) \exp(i\mathbf{q} \cdot \mathbf{R}_{\ell\ell'} - i\omega t), \quad (14)$$

where $\mathbf{q}$ – the wave vector of phonon ($2\pi/\text{wave length}$), $\mathbf{R}_{\ell}$ – the radius vector from zero-reference datum to ℓ -atom, $\mathbf{R}_{\ell\ell'}$ – the vector which is derived from ℓ -atom to ℓ' -atom. Making substitution (2) in the equation (1) we will receive:

$$M\omega^2 = \sum_{\ell'} \Phi_{\alpha\alpha}(\ell, \ell') \exp(i\mathbf{q} \cdot \mathbf{R}_{\ell\ell'}). \quad (15)$$

The last equation can be understood as follows:

$$M\omega^2 = \sum_{n=1}^N \Phi_n \left[1 - \cos \left(\frac{naq}{2} \right) \right], \quad (16)$$

where a is the lattice parameter, $q = |\mathbf{q}|$, Φ_n is the linear combination of $\Phi_{\alpha\alpha}(\ell, \ell')$, for which phase $\mathbf{q} \cdot \mathbf{R}_{\ell\ell'}$ is constant. In fact, Φ_n represents the force between the atom and the plane (there are two, symmetrically arranged), which is perpendicular to $\mathbf{q}$ and is located throughout n of such planes. This sum includes N terms and $\Phi_n = 0$ for $n > N$. If there is long-wave approximation $\mathbf{q} \rightarrow 0$ the difference in the square bracket in equation (4) is converted as

$$1 - \cos \left(\frac{naq}{2} \right) \approx 1 - \left(1 - \frac{1}{2} \left(\frac{naq}{2} \right)^2 \right) = \frac{1}{8} n^2 a^2 q^2.$$

As a result, the equation (16) takes the form:

$$M\omega^2 = \sum_{n=1}^N \frac{1}{8} n^2 a^2 q^2 \Phi_n. \quad (17)$$

The equation (17) in parallel with the Born-Begbie model can be applied to expression of elastic constant for metals and alloys through interplanar force constants Φ_n . According to the Born-Begbie model, it is possible to express

the speed of longitudinal waves in the direction [100] of cubic crystals:

$$v_s = \frac{\omega}{q} = \left(\frac{C_{11}}{\rho} \right)^{\frac{1}{2}}$$

or

$$\rho \omega^2 = C_{11} q^2. \quad (18)$$

For body-centered cubic crystal taking into account $\rho = \frac{2M}{a^3}$, of (5) and (6) we receive:

$$C_{11} = \frac{1}{2a} \sum_{n=1}^N \frac{n^2}{2} \Phi_n. \quad (19)$$

Similarly for transverse waves in the direction [100]

$$C_{44} = \frac{1}{2a} \sum_{n=1}^N \frac{n^2}{2} \Phi_n. \quad (20)$$

Along [110]

$$C_{11} + C_{12} + 2C_{44} = \frac{1}{2a} \sum_{n=1}^N \frac{n^2}{2} \Phi_n. \quad (\text{longitudinal } L \text{ branch}); \quad (21)$$

$$C_{44} = \frac{1}{4a} \sum_{n=1}^N \frac{n^2}{2} \Phi_n. \quad (\text{cross } T_2 \text{ branch}); \quad (22)$$

$$C_{11} - C_{12} = \frac{1}{2a} \sum_{n=1}^N \frac{n^2}{2} \Phi_n. \quad (\text{cross } T_1 \text{ branch}). \quad (23)$$

Along [111]

$$C_{11} + 2C_{12} + 4C_{44} = \frac{1}{2a} \sum_{n=1}^N \frac{n^2}{2} \Phi_n. \quad (\text{longitudinal } L); \quad (24)$$

$$C_{11} - C_{12} + C_{44} = \frac{1}{2a} \sum_{n=1}^N \frac{n^2}{2} \Phi_n. \quad (\text{cross } T). \quad (25)$$

The right parts of the equations (21)-(25) need to be multiplied by two for face-centered cubic structures.

Equation (16) is widely used to describe the phonon spectra using the theoretically calculated force constants $\Phi_{aa}(\ell, \ell')$, as well as in the

estimation of force constant $\Phi_{aa}(\ell, \ell')$ from the experimentally measured phonon spectrum by the least squares method. So in [6], equation (16) is written in the form:

$$M\omega^2 = (4\alpha_1 + 4\beta_2 + 8\alpha_3 + 8\alpha_4 + 4\alpha_5 + 4\gamma_5)(1 - \cos\pi\zeta) + \\ + (2\beta_2 + 8\beta_3 + 4\alpha_4 + 4\beta_4)(1 - \cos 2\pi\zeta) + \\ + (4\beta_5 + 4\gamma_5)(1 - \cos 3\pi\zeta), \quad (26)$$

for lead with the FCC structure in the direction of $[\zeta 00]$ including five planes and the fact that $q = 2\pi\zeta/a$ and $\zeta \in [0, 1]$.

Using (26) and the experimentally measured lead's phonon spectrum is found by least squares method force constants in the first coordination sphere – $\alpha_1 \sim 4 \times 10^3$ dyne/cm and $\beta_1 \sim -2 \times 10^3$ dyne/cm. As the authors [6], using this method to estimate the force constants for distant spheres, the significance of the result is lost. The interplanar force constants Φ_n , for the first eight neighboring planes, are calculated in [6] from lead's phonon spectrum, measured in the direction of symmetry. It is also indicated that the values of Φ_n do not depend on the number of registered planes in the sum of equation (16).

Following the above mentioned method in [7], using the equations (20)-(25) from the experimentally measured phonon spectrum $\alpha\text{-Fe}$ [8], the interplanar force constants Φ_n , elastic constants and their combinations, which are shown in **Table 1** by comparing with the experimental values [9], are calculated. Apparently, two-three first terms, except for the equation (24), where the description of the sum of $C_{11} + 2C_{12} + 4C_{44}$ is required, is enough. Seven terms of Φ_n is enough for consensus

Table 1

Calculations results of interplanar force constants, elastic constants and their combinations of the single crystal $\alpha\text{-Fe}$ from the phonon spectrum [7]

Directions	Interplanar force constants (N/m)							Elastic constants and their combinations (10^{10} N/m ²)	
	Φ_1	Φ_2	Φ_3	Φ_4	Φ_5	Φ_6	Φ_7	Calculation	Experiment [9]
[100]L	138.8	34.3						$C_{11} = 24.6$	$C_{11} = 23.31$
[100]T	134.0	-0.5						$C_{44} = 11.53$	$C_{44} = 11.78$
[110]L	-53.9	184.7						$C_{11} + C_{12} + 2C_{44} = 59.75$	$C_{11} + C_{12} + 2C_{44} = 60.41$
[110]T ₂	-62.7	113.8	-13.7					$C_{44} = 11.75$	$C_{44} = 11.78$
[111]L	44.3	30.8	91.8	6.3	1.8	-0.06	-0.52	$C_{11} + 2C_{12} + 4C_{44} = 97.06$	$C_{11} + 2C_{12} + 4C_{44} = 97.51$
[111]T	127.8	29.0						$C_{11} - C_{12} + C_{44} = 21.27$	$C_{11} - C_{12} + C_{44} = 21.58$

achievement of calculation results of elastic constants with experiment in the right parts of the equations. Here we can conclude that the first two-three harmonicas is enough for the description of dispersive curves α -Fe in the directions [100] and [110] with application of the formula (16). The first seven harmonicas are necessary for the description of longitudinal branch [111]. Therefore, the authors [7] noticed that this branch can be the most informative for force constants calculations of α -iron.

In [10] the conclusion of dynamic matrix for FCC crystals, given in the Born-Karman model, the formula similar to the formula (16) is developed, and the following ratios between elastic constants and force constants in the first three coordination spheres are written:

$$\begin{aligned}\alpha C_{11} &= 4\alpha_1 + 4\alpha_2 + 16\alpha_3 + 8\beta_3; \\ \alpha C_{44} &= 2\alpha_1 + 2\beta_1 + 4\beta_2 + 4\alpha_3 + 20\beta_3; \\ \alpha(C_{11} + C_{44}) &= 4\gamma_1 + 8\gamma_3 + 32\delta_3;\end{aligned}\quad (27)$$

B. Warren noted that elastic constants and dispersions of elastic waves are expressed in the theory of Born-Karman through interatomic force constants. Therefore from curves $\omega(q)$ of elastic waves for three directions, received from measurements of thermal diffuse of X-rays scattering with use of ratios (27), it is possible to receive numerical values of nine independent force constants. This method is applied for aluminum in work [11] which results are given in **Table 2**. There are force constants A_p derived from a phonon spectrum in [3], and also calculated by a pseudopotential method in [12] are given in the same place for comparison. Except β_2 , α_3 and γ_3 , the satisfactory consent of the compared results is observed.

In [3] the phonon spectrum of aluminum is experimentally investigated at temperatures of 80K and 300K and the analysis in the Born-Karman model with use axisymmetric force constants in the first eight coordination spheres. Using the derived force constants, density function of phonon states $g(\omega)$ and thermodynamic properties of aluminum are calculated. The calculated dependence of

Table 2
Born-Karman force constants for aluminum (10^{-3} N/m).

Born-Karman force constants	[11]	[3]	[12]
α_1	8450	10107	9769.6
β_1	-930	-1337	-87.6
γ_1	10670	11444	9857.2
α_2	2140	2454	1781.8
β_2	400	-529	8.2
α_3	270	-625	-887.3
β_3	-310	-182	-149.9
γ_3	100	-296	-491.5
δ_3	-190	-148	-245.7

specific heat on temperature is coordinated with experiment in the range of temperatures from 20K to 80K. Such behavior was also revealed for Debye-Waller's factor. It was concluded that the data of inelastic neutron scattering and calculated thermodynamic properties are consistent at low temperatures, at which the deviation from the quasi-harmonic approximations are small.

5. DYNAMICAL MATRIXES OF FCC METALS AND THEIR RELATION TO ELASTIC CONSTANTS

Dynamical matrix $\mathbf{D}(\mathbf{q})$, in case of the face centered cubic crystal lattices, has dimension 3x3. Its elements $D_{\alpha\beta}(\mathbf{q})$ in the De Launay model, taking into account radial α_n and tangential β_n ($n = 1, \dots, 10$) of the force constants for the first ten coordination spheres, have the form [13]:

$$\begin{aligned}D_{11} &= 2(\alpha_1 + \beta_1)(2 - C_1 C_2 - C_1 C_3) + 4\beta_1(1 - C_2 C_3) + 2(\alpha_2 - \beta_2)(1 - C_{21}) + 2\beta_2(3 - C_{21} - C_{22} - C_{23}) + (4/3)(\alpha_3 - \beta_3)(6 - C_1 C_2 C_{23} - C_1 C_{22} C_3 - 4C_{21} C_2 C_3) + 8\beta_3(3 - C_1 C_2 C_{23} - C_1 C_{22} C_3 - C_{21} C_2 C_3) + 2(\alpha_4 - \beta_4)(2 - C_{21} C_{22} - C_{21} C_{23}) + 4\beta_4(3 - C_{21} C_{22} - C_{21} C_{23} - C_{22} C_{23}) + (18/3)(\alpha_5 - \beta_5)(2 - C_{31} C_2 - C_{31} C_3) + (2/5)(\alpha_5 - \beta_5)(2 - C_1 C_{32} - C_1 C_{33}) + 4\beta_5(6 - C_{31} C_2 - C_{31} C_3 - C_1 C_{32} - C_1 C_{33} - C_{32} C_3 - C_2 C_{33}) + (8/3)(\alpha_6 - \beta_6)(1 - C_{21} C_{22} C_{23}) + 8\beta_6(1 - C_{21} C_{22} C_{23}) + (36/7)(\alpha_7 - \beta_7)(2 - C_{31} C_{22} C_3 - C_{31} C_2 C_{23}) + (16/7)(\alpha_7 - \beta_7)(2 - C_{21} C_{32} C_3 - C_{21} C_2 C_{33}) + (4/7)(\alpha_7 - \beta_7)(2 - C_1 C_{22} C_{33} - C_1 C_{32} C_{23}) + 8\beta_7(6 - C_{31} C_{22} C_3 - C_{31} C_2 C_{23} - C_{21} C_{32} C_3 - C_{21} C_2 C_{33} - C_1 C_{22} C_{33} - C_1 C_{32} C_{23}) + 2(\alpha_8 - \beta_8)(1 - C_{41}) + 2\beta_8(3 - C_{41} - C_{42} - C_{43}) + (4/9)(\alpha_9 - \beta_9)(2 - C_1 C_2 C_{43} - C_1 C_{42} C_3) + (64/9)(\alpha_9 - \beta_9)(1 - C_{41} C_2 C_3) + 8\beta_9(3 - C_1 C_2 C_{43} - C_1 C_{42} C_3 - C_{41} C_2 C_3) + 2(\alpha_9 - \beta_9)(2 - C_{31} C_{32} - C_{31} C_{33}) + 4\beta_9(3 - C_{31} C_{32} - C_{31} C_{33} - C_{32} C_{33}) + (4/5)(\alpha_{10} - \beta_{10})\end{aligned}$$

$$(2-C_{21}C_{42}-C_{21}C_{43}) + (16/5)(\alpha_{10}-\beta_{10})(2-C_{41}C_{22}-C_{41}C_{23}) + 4\beta_9(6-C_{21}C_{42}-C_{21}C_{43}-C_{41}C_{22}-C_{41}C_{23}-C_{22}C_{43}-C_{42}C_{23}). \quad (28)$$

$$\begin{aligned} D_{12} = & 2(\alpha_1-\beta_1)S_1S_2 + (4/3)(\alpha_3-\beta_3)(S_1S_2C_{23} + 2S_1S_{22}C_3 + 2S_{21}S_2C_3) \\ & + (\alpha_4-\beta_4)S_{21}S_{22} + (6/5)(\alpha_5-\beta_5)(S_{31}S_2-S_1S_{32}) + (8/3) \\ & (\alpha_6-\beta_6)S_{21}S_{22}C_{23} + (24/7)(\alpha_7-\beta_7)(S_{31}S_{22}C_3-S_{21}S_{32}C_3) \\ & + (8/7)(\alpha_7-\beta_7)(S_{21}S_2C_{33} + S_{22}S_1C_{33}) + (12/7)(\alpha_7-\beta_7) \\ & (S_1S_{32}C_{23} + S_2S_{31}C_{23}) + 2(\alpha_9-\beta_9)S_{31}S_{32} + (4/9)(\alpha_9-\beta_9) \\ & S_1S_2C_{43} + (16/9)(\alpha_9-\beta_9)(S_{41}S_2C_3 + S_1S_{42}C_3) + (8/5) \\ & (\alpha_{10}-\beta_{10})(S_{21}S_{42}-S_{41}S_{22}), \end{aligned} \quad (29)$$

where $C_i = \cos(aq_i/2)$, $S_i = \sin(aq_i/2)$, $C_{2i} = \cos aq_i$, $S_{2i} = \sin aq_i$, $C_{3i} = \cos(3aq_i/2)$, $S_{3i} = \sin(3aq_i/2)$, $C_{4i} = \cos 2aq_i$, $S_{4i} = \sin 2aq_i$, $i = 1, 2, 3$.

Long-wave approximation is applied to calculate the elastic constants using the elements of the dynamical matrix $D(q)$. As a result of the limit process when $q \rightarrow 0$, the following relations are obtained [13]:

$$\begin{aligned} C_{11} = & \frac{1}{a}(2\alpha_1 + 2\beta_1 + 4\alpha_2 + 12\alpha_3 + 12\beta_3 + 8\alpha_4 + 8\beta_4 + \\ & + \frac{164}{5}\alpha_5 - \frac{328}{5}\beta_5 + \frac{16}{3}\alpha_6 + \frac{32}{3}\beta_6 + 56\alpha_7 + 56\beta_7 + 32\alpha_8 - \\ & - 16\beta_8 + \frac{226}{3}\alpha_9 - \frac{136}{3}\beta_9 + \frac{256}{5}\alpha_{10} + \frac{144}{5}\beta_{10}). \end{aligned} \quad (30)$$

$$\begin{aligned} C_{12} = & \frac{1}{a}(\alpha_1 - 5\beta_1 - 4\beta_2 + 6\alpha_3 - 30\beta_3 + 4\alpha_4 - 20\beta_4 + \\ & + \frac{54}{5}\alpha_5 + 22\beta_5 + \frac{16}{3}\alpha_6 - \frac{64}{3}\beta_6 - \frac{268}{7}\alpha_7 + \frac{124}{7}\beta_7 - \\ & - 16\beta_8 + \frac{49}{3}\alpha_9 - \frac{139}{3}\beta_9 + 80\beta_{10}). \end{aligned} \quad (31)$$

$$\begin{aligned} C_{44} = & \frac{1}{a}(\alpha_1 + 3\beta_1 + 4\alpha_2 + 6\alpha_3 + 18\beta_3 + 4\alpha_4 + 12\beta_4 + \\ & + \frac{18}{5}\alpha_5 - \frac{182}{5}\beta_5 + \frac{16}{3}\alpha_6 + \frac{32}{3}\beta_6 + 28\alpha_7 + 84\beta_7 + \\ & + 16\beta_8 + \frac{49}{3}\alpha_9 - \frac{41}{3}\beta_9 + \frac{64}{5}\alpha_{10} + \frac{336}{5}\beta_{10}). \end{aligned} \quad (32)$$

These expressions allow, for the values of the radial and tangential force constants, to carry our calculation of the elastic constants of metals and alloys with face-centered cubic lattice.

6. DYNAMICAL MATRIXES OF BCC METALS AND THEIR RELATION TO ELASTIC CONSTANTS

According to De Launay model in [14] $D_{ij}(q)$ dynamic matrix elements, taking into account interaction in the first three coordination spheres through "bond-stretching" – A_n and

"bond-bending" – B_n ($n = 1, 2, 3$) force constants, are written down for BCC structures:

$$\begin{aligned} D_{ii} = & \frac{8}{3}A_i(1 - C_iC_jC_k) + 2A_2(1 - C_{2i}) + \\ & + 4A_3(2S_i^2 + S_j^2 + S_k^2 - 2S_i^2S_j^2 - 2S_j^2S_k^2) + \\ & + 8B_1(1 - C_iC_jC_k) + 2B_2(3 - C_{2i} - C_{2j} - C_{2k}) + \\ & + 16B_3(S_i^2 + S_j^2 + S_k^2 - S_i^2S_j^2 - S_j^2S_k^2 - S_i^2S_k^2). \end{aligned} \quad (33)$$

$$D_{ij} = \frac{8}{3}A_iS_iS_jC_k + 8A_3S_iS_jC_k,$$

where $C_i = \cos((1/2)aq_i)$, $S_i = \sin((1/2)aq_i)$, $C_{2i} = \cos(aq_i)$, $i = 1, 2, 3$ and value 1 corresponds to the axis x , value 2 to axis y , value 3 to axis z . Pay attention that we use $A_n = \alpha_n - \beta_n$ and $B_n = \beta_n$ for designation of radial and tangential constants.

In the conception of axially symmetric forces in [14] the correlations between the elastic constants C_{11} , C_{12} , C_{44} and force constants A_1 , A_2 , B_1 , B_2 for BCC metals:

$$\begin{aligned} aC_{11} = & \frac{2}{3}A_1 + 2A_2 + 2B_1 + 2B_2; \\ aC_{12} = & \frac{2}{3}A_1 - 2B_1 - 2B_2; \\ aC_{44} = & \frac{2}{3}A_1 + 2B_1 + 2B_2. \end{aligned} \quad (34)$$

The values of the three force constants were calculated from equations (34) and the fourth value is the frequency ν_T of the transverse phonon mode in the direction [100] at the boundary zone:

$$4\pi^2 m \nu_T^2 = \frac{16}{3}(A_1 + 3B_1),$$

where m is the mass of atom.

Using the abovementioned method, the authors [14] have calculated A_1 , A_2 , B_1 , B_2 via corresponding experimental values of C_{11} , C_{12} , C_{44} and ν_T of each metals for the alkali metals Li , Na , K and Rb . Extending axially symmetric model and taking into account six types of force constants A_1 , A_2 , A_3 , B_1 , B_2 , B_3 , the authors [14] have calculated phonon spectra of the considered metals and have concluded that, in general, measurement of the interatomic interactions up to the third sphere does not improve the description of the phonon spectrum of alkali metals, and this indicates the dominance of the two-particle interaction in these metals.

Compact formulas for the calculations of the elastic constants C_{11} , C_{12} for the BCC metals using derivatives of the pair potential of interatomic interaction $V(r)$ offered in [15]:

$$C_{11} = (6\Omega_0)^{-1} \sum_{l,\alpha} x_\alpha^4(n) \left[\frac{d^2 V}{dR^2} - \frac{1}{R} \frac{dV}{dR} \right]_{R=R_n}; \quad (35)$$

$$C_{12} = (6\Omega_0)^{-1} \sum_{l,\alpha \neq \beta} x_\alpha^2(n) x_\beta^2(l) \left[\frac{d^2 V}{dR^2} - \frac{1}{R} \frac{dV}{dR} \right]_{R=R_n}, \quad (36)$$

where Ω_0 is the atomic volume; R_n is the radius of the n th-coordination sphere; indexes α and β can take the values 1, 2, 3, and the value 1 corresponds to the x -axis, the value 2 to y axis, value 3 to z axis. The designation $x_\alpha^2(n)$ corresponds to the projection on the axis α of the atom, located in the n coordination sphere. The prime mark near index of summation means that sum with $n = 0$ is excluded.

It is possible to apply a ratio [15]:

$$\bar{\omega}^2 = a \frac{2C_{44} + C_{11}}{M}, \quad (37)$$

for calculation of elastic constants C_{44} value, where $\bar{\omega}^2$ is the second moment of phonon frequencies; a is lattice parameter; M is atomic mass. The second moment of phonon frequencies is expressed through derivatives of pair potential $V(r)$ as follows [15]:

$$\bar{\omega}^2 = (3M)^{-1} \sum_n N_n \left(2 \frac{dV}{RdR} + \frac{d^2 V}{dR^2} \right)_{R=R_n}. \quad (38)$$

Here, N_n is atoms' number on n -coordination sphere of R_n radius.

The first and second derivatives of pair potential $V(r)$, which are radial and tangential force constants, as well as in the formula (2), appear in expressions (35), (36) and (38):

$$\alpha_n = \left(\frac{d^2 V}{dR^2} \right)_{R_n}; \beta_n = \left(\frac{dV}{RdR} \right)_{R_n}. \quad (39)$$

The described method was applied to calculate elastic constant of alkaline metals, but they have been able to calculate successfully only C_{12} value for potassium, rubidium and caesium [16].

In De Launay model with application of formulas (9) it is possible to describe elements of dynamical matrix for BCC structure through

force constants in the first ten coordination spheres α_n and β_n ($n = 1, 10$) as follows [17]:

$$\begin{aligned} D_{11} = & 8\beta_1(1-C_{11}C_{12}C_{12}) + (8/3)(\alpha_1-\beta_1)(1-C_{11}C_{12}C_{13}) + \\ & 2\beta_2(3-C_{21}-C_{22}-C_{23}) + 2(\alpha_2-\beta_2)(1-C_{21}) + 4\beta_3(3-C_{21}C_{22}- \\ & C_{21}C_{23}-C_{22}C_{23}) + 2(\alpha_3-\beta_3)(2-C_{21}C_{22}-C_{21}C_{23}) + 8\beta_4(3- \\ & C_{31}C_{12}C_{13}-C_{11}C_{32}C_{13}-C_{11}C_{12}C_{33}) + (\alpha_4-\beta_4)[(72/11) \\ & (1-C_{31}C_{12}C_{13}) + (8/11)(2-C_{11}C_{32}C_{13}-C_{11}C_{12}C_{33})] + 8\beta_5(1- \\ & C_{12}C_{22}C_{23}) + (8/3)(\alpha_5-\beta_5)(1-C_{21}C_{22}C_{23}) + 2\beta_6(3-C_{41}- \\ & C_{42}-C_{43}) + 2(\alpha_6-\beta_6)(1-C_{41}) + 8\beta_7(3-C_{31}C_{32}C_{13}-C_{31}C_{12}C_{33}- \\ & C_{11}C_{32}C_{33}) + (\alpha_7-\beta_7)[(8/19)(1-C_{11}C_{32}C_{33}) + (72/19) \\ & (2-C_{31}C_{32}C_{13}-C_{31}C_{12}C_{33})] + 4\beta_8(6-C_{41}C_{22}-C_{41}C_{23}- \\ & C_{21}C_{42}-C_{21}C_{43}-C_{42}C_{23}-C_{22}C_{43}) + 4(\alpha_8-\beta_8)[(4/5) \\ & (2-C_{41}C_{22}-C_{41}C_{23}) + (1/5)(2-C_{21}C_{42}-C_{21}C_{43})] + 8\beta_9(3- \\ & C_{41}C_{22}C_{23}-C_{21}C_{22}C_{43}-C_{21}C_{42}C_{23}) + 8(\alpha_9-\beta_9)[(2/3) \\ & (1-C_{41}C_{22}C_{23}) + (1/6)(2-C_{21}C_{22}C_{43}-C_{21}C_{42}C_{23})] + 8\beta_{10}(1- \\ & C_{31}C_{32}C_{33}) + (8/3)(\alpha_{10}-\beta_{10})(1-C_{31}C_{32}C_{33}) + 8\beta_{10}(3- \\ & C_{51}C_{12}C_{13}-C_{11}C_{52}C_{13}-C_{11}C_{12}C_{53}) + (\alpha_{10}-\beta_{10})[(200/27) \\ & (1-C_{51}C_{12}C_{13}) + (8/27)(2-C_{11}C_{52}C_{13}-C_{11}C_{12}C_{53})]; \quad (40) \end{aligned}$$

$$\begin{aligned} D_{12} = & (8/3)(\alpha_1-\beta_1)S_{11}S_{12}C_{13} + 2(\alpha_3-\beta_3)S_{21}S_{22} + 8(\alpha_4-\beta_4) \\ & [(1/11)S_{11}S_{12}C_{33} + (3/11)(S_{31}S_{12}C_{13} + S_{11}S_{32}C_{13})] + (8/3) \\ & (\alpha_5-\beta_5)S_{21}S_{22}C_{23} + 8(\alpha_7-\beta_7)[(9/19)S_{31}S_{32}C_{13} + (3/19) \\ & (S_{31}S_{12}C_{33} + S_{11}S_{32}C_{33})] + (8/5)(\alpha_8-\beta_8)(S_{41}S_{22} + S_{21}S_{42}) + \\ & 8(\alpha_9-\beta_9)[(1/6)S_{21}S_{22}C_{43} + (1/3)(S_{41}S_{22}C_{23} + S_{21}S_{42}C_{23})] \\ & + (8/3)(\alpha_{10}-\beta_{10})S_{31}S_{32}C_{33} + 8(\alpha_{10}-\beta_{10})[(1/27) \\ & S_{11}S_{12}C_{53} + (5/27)(S_{51}S_{12}C_{13} + S_{11}S_{52}C_{13})], \quad (41) \end{aligned}$$

where $C_i = \cos(aq_i/2)$, $S_i = \sin(aq_i/2)$, $C_{2i} = \cos(aq_i)$, $S_{2i} = \sin(aq_i)$, $C_{3i} = \cos(3aq_i/2)$, $S_{3i} = \sin(3aq_i/2)$, $C_{4i} = \cos(2aq_i)$, $S_{4i} = \sin(2aq_i)$, $C_{5i} = \cos(5aq_i/2)$, $S_{5i} = \sin(5aq_i/2)$, $i = 1, 2, 3$ and a – lattice parameter.

There are elements of D_{ij} dynamical matrix in the directions [100], [001], [110] in space $\mathbf{q}$ and they are compared with similarly recorded elements of dynamic matrix in the Born-Begbie model for deriving expressions for the elastic constants C_{11} , C_{12} , C_{14} in the long wavelength approximation ($q \rightarrow 0$). As a result, we receive the following expression [17]:

$$c_{11} = \frac{1}{a} \left[\frac{4}{3}\alpha_1 + \frac{8}{3}\beta_1 + 4\alpha_2 + 8\alpha_3 + 8\beta_3 + \frac{332}{11}\alpha_4 + \frac{152}{11}\beta_4 + \right. \\ \left. + \frac{16}{3}\alpha_5 + \frac{32}{3}\beta_5 + 16\alpha_6 + \frac{652}{19}\alpha_7 + \frac{792}{19}\beta_7 + \right. \\ \left. + \frac{272}{5}\alpha_8 + \frac{128}{5}\beta_8 + 48\alpha_9 + 48\beta_9 + 12\alpha_{10} + 12\beta_{10} \right];$$

$$\begin{aligned} c_{12} = & (1/a)(4\beta_1-4\beta_2-16\beta_3-44\beta_4-16\beta_5-16\beta_6-76\beta_7-8\beta_8-96\beta_9-36\beta_{10}); \\ c_{44} = & \frac{1}{a} \left[\frac{4}{3}\alpha_1 + \frac{8}{3}\beta_1 + 4\beta_2 + 4\alpha_3 + 12\beta_3 + \frac{76}{11}\alpha_4 + \frac{408}{11}\beta_4 + \right. \\ & \left. + \frac{16}{3}\alpha_5 + \frac{32}{3}\beta_5 + 16\beta_6 + \frac{316}{19}\alpha_7 + \frac{1048}{19}\beta_7 + \right. \\ & \left. + \frac{64}{5}\alpha_8 + \frac{336}{5}\beta_8 + 24\alpha_9 + 72\beta_9 + 12\alpha_{10} + 24\beta_{10} \right]. \quad (42) \end{aligned}$$

Approbation of these expressions is performed in [17] by calculations of the elastic constants of alkali metals using pseudopotential method when compared with the experimental data.

7. THE GENERAL FORMULA FOR CALCULATIONS OF THE DYNAMICAL MATRIX AND THE ELASTIC CONSTANTS OF THE BCC AND FCC STRUCTURES

G. Squires [2] offered the general formula to calculate dynamical matrix elements of *FCC* and *BCC* crystals through force constants of Born-Karman in the form:

$$A_{ii} = \frac{8}{M} \sum_s \frac{n^s}{48} \sum_j \alpha_j^s \{2 - C_{j,i}^s [C_{j+1,i+1}^s C_{j+2,i+2}^s + C_{j+2,i+1}^s C_{j+1,i+2}^s]\};$$

$$A_{i,i+1} = \frac{8}{M} \sum_s \frac{n^s}{48} \sum_j \beta_j^s C_{j,i+2}^s [S_{j+1,i}^s S_{j+2,i+1}^s + S_{j+2,i}^s S_{j+1,i+1}^s], \quad (43)$$

where α_j^s and β_j^s are force constants by definition (1), $C_{j,i}^s = \cos(\pi a h_j^s q_i)$, $S_{j,i}^s = \sin(\pi a h_j^s q_i)$, a is lattice parameter, h_j^s are atom coordinates in s -th coordination sphere (3), $i = 1, 2, 3$ and when $i + 1$ more than 3, it corresponds to $i - 2$, in the similar case $i + 2$ corresponds to $i - 1$, the same kind of thing for j index.

Ratio between interatomic force constants and elastic constants C_{11} , C_{12} and C_{44} turns out as $|\mathbf{q}|$ tends to zero and A_{ij} matrix equating with matrix of elastic waves in a continuum [2]. These ratios have the form for *FCC* structure:

$$aC_{11} = 8 \sum_s \frac{n^s}{48} \sum_j (h_j^s)^2 \alpha_j^s;$$

$$aC_{44} = 4 \sum_s \frac{n^s}{48} \sum_j [(h_{j+1}^s)^2 + (h_{j+2}^s)^2] \alpha_j^s; \quad (44)$$

$$a(C_{12} + C_{44}) = 16 \sum_s \frac{n^s}{48} \sum_j h_{j+1}^s h_{j+2}^s \beta_j^s.$$

The results of C_{11} , C_{12} , C_{44} calculations should be divided by 2 for *BCC* structure. The last expressions are used while calculating elastic constant of *BCC* and *FCC* metals and alloys when values of force constants in the Born-Karman model are known.

Within De Launay model, the given formulas, (28) and (40), (29) and (41), for elements of dynamical matrix of *BCC* and *FCC* structures, are respectively generalized and presented in the form [18]:

$$D_{11} = \frac{1}{6} \sum_n N_n \left\{ \frac{\beta_n [6 - C_{h1} C_{k2} C_{l3} - C_{h1} C_{l2} C_{k3} - C_{k1} C_{h2} C_{l3} - C_{k1} C_{l2} C_{h3} - C_{l1} C_{h2} C_{k3} - C_{l1} C_{h2} C_{h3}] + \frac{\alpha_n - \beta_n}{h^2 + k^2 + l^2} [h^2 (2 - C_{h1} C_{k2} C_{l3} - C_{h1} C_{l2} C_{k3}) + k^2 (2 - C_{k1} C_{h2} C_{l3} - C_{k1} C_{l2} C_{h3}) + h^2 (2 - C_{l1} C_{h2} C_{k3} - C_{l1} C_{k2} C_{h3})]} \right\}; \quad (45)$$

$$D_{11} = D_{22} = D_{33}.$$

$$D_{12} = \frac{1}{6} \sum_n N_n \frac{\alpha_n - \beta_n}{h^2 + k^2 + l^2} \left[\frac{hk(S_{h1} S_{k2} C_{l3} + S_{k1} S_{h2} C_{l3}) + hl(S_{h1} S_{h2} C_{k3} + S_{l1} S_{h2} C_{k3}) + kl(S_{k1} S_{l2} C_{h3} + S_{l1} S_{k2} C_{h3})}{h^2 + k^2 + l^2} \right]; \quad (46)$$

$$D_{12} = D_{23} = D_{13}.$$

where N_n is number of atoms in n -coordination sphere, the set h, k, l are coordinates of atoms, as in the formula (3), $C_{hj} = \cos(h a q_j / 2)$, $C_{kj} = \cos(k a q_j / 2)$, $C_{lj} = \cos(l a q_j / 2)$, $S_{hj} = \sin(h a q_j / 2)$, $S_{kj} = \sin(k a q_j / 2)$, $S_{lj} = \sin(l a q_j / 2)$, $j = 1, 2, 3$ ($q_1 = q_x$; $q_2 = q_y$; $q_3 = q_z$), a - lattice parameter.

There are elements of D_{ij} of dynamical matrix in the directions [100], [001], [110] in space q and they are compared with similarly recorded elements of dynamical matrix in the Born-Begbie model for deriving expressions for the elastic constants C_{11} , C_{12} , C_{44} in the long wavelength approximation $q \rightarrow 0$. As a result, we receive for *BCC* structure [18]:

$$C_{11} = \frac{1}{12a} \sum_i N_i \left\{ \beta_i (h^2 + k^2 + l^2) + [\alpha_i - \beta_i] \frac{h^4 + k^4 + l^4}{h^2 + k^2 + l^2} \right\};$$

$$C_{44} = \frac{1}{12a} \sum_i N_i \left\{ \beta_i (h^2 + k^2 + l^2) [\alpha_i - \beta_i] \frac{h^2 k^2 + h^2 l^2 + k^2 l^2}{h^2 + k^2 + l^2} \right\}; \quad (47)$$

$$C_{12} + C_{44} = \frac{1}{6a} \sum_i N_i [\alpha_i - \beta_i] \frac{h^2 k^2 + h^2 l^2 + k^2 l^2}{h^2 + k^2 + l^2}.$$

The results of C_{11} , C_{12} , C_{44} calculations should be multiplied by 2 for *FCC* structure.

Formula's certainty (47) was checked in [18] by calculations of elastic constant for alkaline and some transition metals by pseudopotential method when comparing with experimental data.

8. CALCULATION FOR FORCE AND ELASTIC CONSTANTS OF FCC AND BCC METALS USING PSEUDOPOTENTIAL

One of the most successfully used model potentials in calculation of physical properties of metals and alloys is the model potential of the Heyne-Abarenkov-Animalu (HAA) [19-21] which parameters are selected with use of experimental information on energy levels of free atoms and ions [22]. According to [19] the ion's potential is defined by means of expressions

$$\begin{aligned} v^{\text{ion}} &= -A_l \text{ при } r < R_m, \\ v^{\text{ion}} &= -(Z/r) \text{ при } r > R_m, \end{aligned} \quad (48)$$

where R_m is the model radius, Z is the ionic valency, A_l is the hole's depth, l is orbital quantum number, v^{ion} is the interaction potential of conduction electron with ion.

Matrix elements of form factors in pseudopotential model of Heyne-Abarenkov-Animalu were calculated in [19-21] for simple elements

$$W^{\text{bare}} = \frac{B(q)}{\varepsilon(q)} + F(q, \vec{k}, \vec{k}') + I(\vec{q}), \quad (49)$$

where $B(q)$ – local part:

$$\begin{aligned} B(q) &= \frac{-8\pi A_2}{\varepsilon(q)} [\sin(qR_m) - qR_m \cos(qR_m)] - \frac{8\pi Z}{\Omega q^2} \cos(qR_m) + \\ &+ \left(\frac{4\pi |E_c|}{\Omega q^3} - \frac{24\pi Z \alpha_{\text{eff}}}{\Omega q^2 (qR_c)^3} \right) [\sin(qR_c) - qR_m \cos(qR_c)], \end{aligned} \quad (50)$$

$F(q, \vec{k}, \vec{k}')$ – not local part:

for $\vec{k} = \vec{k}'$

$$\begin{aligned} F(q, \vec{k}, \vec{k}') &= -\frac{4\pi R_m^3}{\Omega} (A_0 - A_2) \left\{ j_0^2(kR_m) - \frac{\cos(kR_m)}{kR_m} j_1(kR_m) \right\} - \\ &- \frac{12\pi R_m^3}{\Omega} (A_1 - A_2) \left(1 - \frac{q^2}{2k^2} \right) \{ j_1^2(kR_m) - j_0(kR_m) j_2(kR_m) \}, \end{aligned}$$

for $\vec{k} \neq \vec{k}'$

$$\begin{aligned} F(q, \vec{k}, \vec{k}') &= -\frac{8\pi R_m^2}{\Omega(k^2 - k'^2)} (A_0 - A_2) \{ k j_1(kR_m) j_0(k'R_m) - k' j_1(k'R_m) j_0(kR_m) \} - \\ &- \frac{24\pi R_m^2}{\Omega(k^2 - k'^2)} (A_1 - A_2) \left(\frac{k^2 + k'^2 - q^2}{2kk'} \right) \{ k j_2(kR_m) j_1(k'R_m) - k' j_2(k'R_m) j_1(kR_m) \}, \end{aligned}$$

$I(q)$ – integral from not local part:

$$I(q) = -\frac{32m^* [1 - f(q)] (1 + \alpha_{\text{vso}})}{\pi \Omega q^2 \varepsilon(q)} [(A_0 - A_2) L_0 + 3(A_1 - A_2) L_2] R_m^2,$$

$$\begin{aligned} L_l &= \int_{k < k_F} \frac{[k j_{l+1}(kR_m) j_l(k'R_m) - k' j_{l+1}(k'R_m) j_l(kR_m)] P_l(\cos \theta_{kk'}) d^3 k}{k^2 - k'^2}, \\ x &= k_F R_m, \quad \vec{k}' = |\vec{k}_F + \vec{q}| R_m, \quad \cos \theta_{kk'} = \frac{k^2 + k'^2 - (qR_m)^2}{2kk'}. \end{aligned}$$

For transition metals in [21] it was offered to use the following expressions for calculation of form factor of screened pseudopotential model (MPPM of Animalu)

$$W = \frac{B(q) + F(\vec{k}_F, \vec{k}_F + \vec{q})}{\varepsilon(q)}, \quad (51)$$

where $B(q)$ has the same form, as (50), and other terms in (51) are written down in quasilocal approximation:

for $|\vec{k}_F + \vec{q}| = \vec{k}_F$

$$\begin{aligned} F(\vec{k}_F, \vec{k}_F + \vec{q}) &= -\frac{4\pi R_m^3}{\Omega} (A_0 - C) \left\{ j_0^2(x) - \frac{\cos(x)}{x} j_1(x) \right\} - \\ &- \frac{12\pi R_m^3}{\Omega} (A_1 - C) \left(1 - \frac{q^2}{2k^2} \right) \{ j_1^2(x) - j_0(x) j_2(x) \} P_1(\cos \theta) - \\ &- \frac{20\pi R_m^3}{\Omega} (A_2 - C) \{ j_2^2(x) - j_1(x) j_3(x) \} P_2(\cos \theta), \end{aligned}$$

where $x = k_F R_m$, $\cos \theta = 1 - q^2/2k_F^2$, $P_1(\cos \theta) = \cos \theta$, $P_2(\cos \theta) = (3\cos^2 \theta - 1)/2$, $j_0(x) = (\sin x)/x$, $j_1(x) = (\sin x)/x^2 - (\cos x)/x$, $j_2(x) = (3/x^2 - 1/x) \sin x - 3(\cos x)/x^2$.

For $|\vec{k}_F + \vec{q}| \neq \vec{k}_F$

$$\begin{aligned} F(\vec{k}_F, \vec{k}_F + \vec{q}) &= -\frac{8\pi R_m^3}{\Omega(x^2 - y^2)} (A_0 - C) \{ x j_1(x) j_0(y) - y j_1(y) j_0(x) \} - \\ &- \frac{24\pi R_m^3}{\Omega(x^2 - y^2)} (A_1 - C) \{ x j_2(x) j_1(y) - y j_2(y) j_1(x) \} P_1(\cos \theta') - \\ &- \frac{40\pi R_m^3}{\Omega(x^2 - y^2)} (A_2 - C) \{ x j_3(x) j_2(y) - y j_3(y) j_2(x) \} P_2(\cos \theta'), \\ x &= k_F R_m, \quad y = |\vec{k}_F + \vec{q}| R_m, \quad \cos \theta' = [x^2 + y^2 - (qR_m)^2] / (2xy). \end{aligned}$$

Expression (49) is reproduced to the form (51) in quasilocal approximation. Form factors' values tables of the pseudopotentials model, calculated in quasilocal approximation with use of expression (51) for 56 simple and transition elements, are provided in [23].

Within the theory of pseudopotential, the interatomic interaction energy of atoms' crystal can be presented in the form:

$$V(r) = \frac{Z^2 e^2}{r} - \frac{2Ze^2}{\pi} \int_0^\infty G(q) \frac{\sin(qr)}{qr} dq. \quad (52)$$

Here, Z is the valency, e is the electron charge, q is the magnitude of propagation vector, r is interatomic distance, $G(q)$ normalized characteristic function:

$$G(q) = \left[\frac{4\pi Ze^2}{\Omega_0 q^2} \right]^{-2} \frac{W^{\text{bare}}(q)^2}{1-f(q)} (1 - 1/\varepsilon(q)), \quad (53)$$

where $W^{\text{bare}}(q)$ is unscreened ionic potential, Ω is atomic volume,

$$\varepsilon(q) = 1 + [1 - f(q)] \frac{4\pi Ze^2}{\Omega_0 q^2} \left(\frac{2}{3} E_F \right)^{-1} \left[\frac{1}{2} + \frac{4k_F^2 - q^2}{8k_F q} \ln \left| \frac{2k_F + q}{2k_F - q} \right| \right], \quad (54)$$

$E_F = \frac{\hbar^2 k_F^2}{2m^*}$, k_F is Fermi's momentum, m^* is the effective mass of electron, $e^* = (1 + \alpha_{\text{eff}})e$, $f(q)$ is the correction for an exchange and correlation of electrons.

In case of the central interactions, proceeding from the interatomic potential $V(r)$, it is possible to define two types of force constants [12]:

$$\frac{1}{r} \frac{dV}{dr} = -\frac{Z^2 e^2}{\pi r^2} - \frac{2Z^2 e^2}{\pi r^2} \int_0^\infty G(q) \left(\cos qr - \frac{\sin qr}{qr} \right) dq, \quad (55)$$

$$\frac{d^2 V}{dr^2} = -\frac{2Z^2 e^2}{\pi r^2} - \frac{2Z^2 e^2}{\pi r} \int_0^\infty G(q) \left(\frac{2 \sin qr}{qr^2} - \frac{2 \cos qr}{r} - q \sin qr \right) dq. \quad (56)$$

These force constants are designated in the formula (39) as β and α .

In accordance with the above described method with application of MPPM of Animalu, the radial and tangential force constants of transitional *Ni* and *Pd* metals, with the use of which phonon spectra, were developed using dynamical matrix elements, expressed through (28)-(29) and also elastic constants of these metals according to formulas (30)-(32), are calculated in the work [24]. Calculation results [24] of elastic constants *Ni* and *Pd* are given in **Table 3** when comparing with experimental data [25], [26]. These tab. 3 show that nickel's calculation results of [18] elastic constants C_{11} and C_{12} according to the formulas (47) coincide with experiment better [25], than results [24], though in both cases, MPPM of Animalu was used [20] and the values of radial and tangential force constants of nickel, calculated in [18], almost coincide

Table 3
Calculations results of the elastic constants of some metals when compared with the experimental data (10^{10}N/m^2).

Metal	Reference	C_{11}	C_{12}	C_{44}
Ni	[18]	23.25	15.08	8.54
	[24]	22.78	17.84	8.70
	[29]	21.11	19.14	14.48
	Exp.[25]	24.60	15.00	12.20
Pd	[18]	23.48	17.65	6.93
	[24]	24.37	17.57	8.55
	[29]	17.07	13.38	11.42
	Exp.[26]	22.70	17.59	7.17
Cu	[18]	16.68	13.20	9.05
	[33]	16.11	11.82	7.70
	[29]	14.66	12.74	8.03
	Exp.[30,31]	16.84	12.14	7.54
Ag	[18]	12.10	9.74	3.85
	[30]	11.82	10.21	4.99
	[29]	11.52	8.19	5.19
	Exp.[27,28]	12.40	9.37	4.61
Au	[33]	18.88	16.34	4.85
	[29]	14.09	9.07	6.02
	Exp.[21,22]	18.6	15.7	4.20
α -Fe	[34]	24.8	24.8	12.9
	[29]	19.97	19.97	6.58
	[36]	23.0	23.0	12.7
	Exp.[35]	23.31	13.54	11.78
γ -Fe	This paper	15.95	16.49	6.41
	[38]	18.10	18.10	8.32
	[36]	21.0	21.0	13.8
	[37]	15.4	15.4	7.7

with the corresponding values, calculated in [24], that can be seen from **Table 4**. *Pd*'s

Table 4
Radial and tangential force constants *Ni*, (10^{-3}N/m^2).

Number sphere i	[24]		[18]	
	α_i	β_i	α_i	β_i
1	4764.7	-310.6	4762.1	-311.1
2	940.7	72.5	943.9	72.5
3	-163.2	7.4	-164.6	7.4
4	20.5	-0.1	20.7	0.0
5	22.39	0.8	21.9	1.0
6	-13.7	1.2	-13.7	1.3
7	-11.2	-0.1	-11.4	0/0
8	-7.0	-0.3	-7.2	-0.3
9	5.3	-0.3	5.1	-0.3
10	4.6	0.0	4.6	0.1
11	-	-	5.1	-0.2

calculation results the radial and tangential force constants, received in [24] and [18] with application by using MPPM of Animalu, are complied well, and therefore the values of elastic constants, calculated through them, are close to experimental data [26]. The force constants of *Pd*, calculated in [27] where pair interaction of atoms is shown taking into account *s-s*, *d-d*, *s-d* deposits, are given in **Table 5** for comparison. As for superposition of *d* states of the next ions and *s-d* hybridization are considered in approximation [28].

Thus, an effective potential is chosen as a rapidly converging. With such approach, the authors [29] calculated phonon spectrums of *Cu*, *Ag*, *Au*, *Ni*, *Pd*, *Pt* and α -*Fe* in the Born-Karman's model. A good consent between the calculated and experimentally received values of frequencies for normal modes is revealed for all these metals. It may be noted that the calculated phonon spectrum for the *BCC Fe* in the most unsuccessful, as in the [110] direction transverse branches diverge from the experimental branch, and in the [111] a significant discrepancy for longitudinal and lateral modes is also revealed. The Table 3 provides the elastic constants of *Cu*, *Ag*, *Au*, *Ni*, *Pd*, *Pt* and α -*Fe*, calculated by Squires's

formulas (44), taking into account the force constants in the first 32 coordination spheres, which shows that in general the calculated values of elastic constants are consistent with the experimental data.

Success of calculations for elastic constants depends on a choice of model potential. Thus, in [18] we failed to reach agreement with the experimental data [30, 31] for *Cu* with potential HAA [19-21] , but with the potential of Moriarty [32] it was succeeded to approximate to the experimental data that is presented in Tab. 3. Results of calculations of elastic constants for copper by method of a homogeneous deformation with use of bare ionic model potential with one parameter [33] show that the calculated value of *C*₄₄ is closer to the experimental, than result [18] for *C*₄₄. But the HAA potential was suitable for silver proved, as the results [18] for *C*₁₁, *C*₁₂ are closer to the experiment [30, 31] than the calculation results, received with bare ionic potential with one parameter [33]. Results of calculations for elastic constants of *Au* by a method of a homogeneous deformation with use of the potential [33] are in better agreement with the experimental data [30, 31] than the results of the above mentioned work [29]. Elastic constants of α -*Fe*, calculated in [34] by formulas (35)-(38), are presented in Tab. 3 in comparison with the experiment [35] and with calculation results [29], [36]. Radial and tangential force constants of α -*Fe* in the first ten coordination spheres, calculated in [34] with application of the TMMP of Animalu and used in calculations of elastic constants, are given in **Table 6**. Calculation results [34] of elastic constants for α -*Fe*, generally, in good agreement with the experimental data, and are close to the calculation results [36], where it were proceeded from first principles in the local density approximation (*LDA*) within the density functional theory and dynamic theory of an average field, which allows to calculate electronic and structural properties of materials,

Table 5
Radial and tangential force constants Pd,
(10⁻³N/m²)

Number sphere i	[24]		[18]		[27]	
	α_i	β_i	α_i	β_i	α_i	β_i
1	46123.4	-5817.9	45933.6	-5732.3	43169.6	-2240.9
2	1482.9	21.7	1454.9	23.9	-2632.1	269.5
3	-504.3	99.2	-515.4	98.7	162.1	52.4
4	-518.0	-14.6	-501.7	-15.0	-222.1	48.9
5	419.8	-10.6	417.7	-9.9	-225.8	14.5
6	51.4	17.9	46.9	18.0	-8.4	3.8
7	-319.4	2.9	-310.7	2.5	20.1	5.0
8	-28.7	-10.4	-27.4	-10.5	-	-
9	220.6	-2.9	213.7	-2.6	-	-
10	74.3	6.0	72.2	6.2	-	-
11	-	-	-113.5	3.9	-	-

Table 6
 Radial and tangential force constants α -Fe и Re,
 (10^{-3}N/m^2)

Number sphere i	α -Fe [34]		Re [34]	
	α_i	β_i	α_i	β_i
1	63274.0	-6956.0	461452.7	-67507.0
2	15090.0	-1608.0	240034.5	-13643.5
3	-2234.0	237.5	23131.7	-1505.6
4	-5.4	-62.8	-19863.3	824.9
5	894.4	-38.8	-21092.0	-158.0
6	-541.1	31.-	8872.0	367.9
7	-299.2	-22.5	-10709.9	-49.8
8	71.5	-24.4	-5329.2	-264.1
9	278.6	10.3	5191.8	152.2
10	-295.9	7.8	-6296.8	53.9

taking into account correlations of electrons both in paramagnetic and magnetically ordered phases. Thus, the authors [36] calculated a phonon spectrum of γ -Fe in the [100] and [110] directions, having estimated a speed of sound waves; they received values of elastic constants of C_{11} , C_{12} , C_{44} that are shown in Tab. 3. It can be seen that the calculated values of elastic constants exceed the experimental values [37]. The same can be said about the calculation results of elastic constants for α -Fe [38]. Radial and tangential force constants of α -Fe (Table 7), which were applied in calculation of elastic constants [38], are given in [27]. For comparison, the force constants of α -Fe, calculated with use of the TMMP of Animalu, are also given there. It is seen that the compared values are consistent only in the first sphere. With use of force constants, given in Tab. 6, we calculated

Table 7
 Radial and tangential force constants γ -Fe,
 (10^{-3}N/m^2).

Number sphere i	This paper		[27]	
	α_i	β_i	α_i	β_i
1	46963.3	-5135.6	42707.5	-4250.9
2	2314.9	316.5	-886.2	149.9
3	-1951.6	1.4	4.0	45.3
4	1059.5	2.8	-196.6	27.5
5	-581.2	30.0	-89.5	7.3
6	-157.8	-22.8	3.7	4.1
7	-	-	-13.1	3.7

elastic constants of α -Fe and presented them in Tab. 3, which shows that the received values for C_{11} , C_{44} are close to the experimental data.

Formulas (30) for BCC metals and general formulas were approved in [17,18] on an example of alkaline metals Li , Na , K , Rb and Cs by means of calculations of elastic constants with use of the Ashcroft's model potential [39, 40]. Results of these researches are identical and given in Table 8 in comparison with results of other authors and experimental data. On the basis of these data, it can be concluded that the Ashcroft's model potential is suitable for calculation of elastic constants of alkaline metals. In the case of Li , the authors [17] varied a parameter of Ashcroft's potential until receiving of the best convergence of calculation results for elastic constants with the experimental values [41] and chose a value $r_c = 1.284$, with use of which the elastic constants, given in Tab. 8, were received. From this table you can see that values of elastic constants for lithium C_{11} , C_{12} , calculated in [12] by Squires's formulas (44) with use of the Ashcroft's potential,

Table 8
 Calculations results of elastic constants of alkali metals,
 (10^{10}N/m^2)

Metal	Reference	C_{11}	C_{12}	C_{44}
Li	[17, 18]	1.480	1.297	1.056
	[12]	4.055	3.377	1.562
	[42]	1.362	1.151	0.901
	Exp.(78K)[41]	1.486	1.274	1.048
Na	[17, 18]	1.005	0.834	0.633
	[12]	1.008	0.842	0.637
	Exp.(78K)[43]	0.993	0.823	0.560
K	[17, 18]	0.414	0.350	0.262
	[12]	0.413	0.345	0.268
	Exp.(4.2K)[44]	0.416	0.341	0.286
Rb	[17, 18]	0.296	0.259	0.194
	[12]	0.283	0.235	0.190
	Exp.(80K)[45]	0.296	0.250	0.171
Cs	[17, 18]	0.218	0.183	0.142
	[12]	0.221	0.185	0.143
	Exp.(78K)[46]	0.247	0.209	0.148

strongly disagree with experiment that can be explained by the selected parameter value $r_c = 1.678$. Elastic constants of lithium are calculated in [42] using a modified built-in analytical potential, which will be coordinated with experiment [41] more badly than elastic constants, calculated in [17, 18]. The authors [42] didn't specify a calculation method for elastic constants, but they used the Born-Karman's force constants. The Table 8 shows that the calculation results [17, 18] of elastic constants C_{11} , C_{12} , C_{44} for *Na*, *K*, *Rb* and *Cs* are close to the corresponding results [12] and is consistent with experimental data [43-46]. Values of radial and tangential force constants for each of these metals, calculated in [17, 18] and [12] with use of the Ashcroft's model potential, are very similar, as shown by an example of sodium in **Table 9**. The authors [12] converted values of radial and tangential force constants into force constants of the Born-Karman and calculated the elastic constants of *Na*, *K*, *Rb*, and *Cs*, which are given in Table 8, by the Squires's formulas (44). In view of the fact that values of the last agree with the corresponding calculation results by general formulas (47), it is possible to state an adequacy of the formulas (44) and (47).

Table 9

Radial α_i and tangential β_i force constants *Na*,
(10^{-3} H/m).

Number sphere <i>i</i>	β_i		α_i	
	[17, 18]	[12]	[17, 18]	[12]
1	-311.1	-310.6	4762.1	4764.7
2	72.5	72.5	943.9	940.7
3	7.4	7.4	-164.6	-163.2
4	0.0	-0.1	20.7	20.5
5	1.0	0.8	21.9	22.4
6	1.2	1.2	-13.7	-13.7
7	0.0	-0.1	-11.4	-11.2
8	-0.3	-0.3	-7.2	-7.0
9	-0.3	-0.3	5.1	5.3
10	0.08	0.0	4.6	4.6
11	-0.2	-	5.1	-

9. CALCULATION OF ELASTIC CONSTANTS FOR HCP METALS BY THE PSEUDOPOTENTIAL METHOD

As it was noted in [47], for calculation of elastic constants for elements with structure of a hexagonal close packing (*HCP*) in harmonic approximation, we can restrict ourselves to the fourth coordination sphere included. In this approximation, the elastic constants C_{11} , C_{12} , C_{13} , C_{33} and C_{44} can be calculated using the formulas [48, 49]:

$$C_{11} = \frac{\sqrt{3}(3\alpha - A_1 - L)}{2c}, \quad (57)$$

$$C_{12} = C_{11} - \frac{1}{\sqrt{3}c}[3(\alpha - 3A_1) - 3B_1 - B_2 - 12G_1 - 4G_2 + P], \quad (58)$$

$$C_{13} = \frac{2}{a}(2G_4 - B_4) - C_{44}, \quad (59)$$

$$C_{33} = \frac{c}{\sqrt{3}a^2}[-3(B_3 + G_3) + 4\delta], \quad (60)$$

$$C_{44} = -\frac{2}{\sqrt{3}c}(3A_2 + B_3 + 4G_3), \quad (61)$$

$$L = \frac{(2B_2 + G_2 + 3G_1)(3B_1 + B_2 + 8G_2) + 2G_2(3B_1 + B_2)}{3(B_1 + B_2 + G_1 + G_2)},$$

$$P = \frac{(B_1 - B_2 - 2G_1 + 2G_2)^2}{B_1 + B_2 + G_1 + G_2},$$

$$\alpha = -[k_1(1) + C_B(1)], \quad A_1 = A_2 = C_B(1), \quad A_3 = 0,$$

$$B_1 = C_B(2), B_2 = \frac{1}{3}(K_1(2) + 3C_B(2)), B_3 = 2B_2 - B_1, B_4 = \sqrt{2}(B_2 - B_1),$$

$$G_1 = C_B(3), G_2 = \frac{1}{3}(2K_1(3) + 3C_B(3)), G_3 = \frac{1}{2}(G_1 + G_2), G_4 = \frac{G_2 - G_1}{\sqrt{2}},$$

$$\delta = -(K_1(4) + C_B(4)), \quad K_1(S) = (\alpha_i - \beta_i)_s, \quad C_B(S) = (\beta_i)_s.$$

In these formulas, a and c are parameters of a crystal lattice, α_i and β_i ($i = 1, 4$) – tangential and radial force constants.

Calculations of elastic constant of *Mg*, *Zr*, and *Ti* with *HCP* structure were carried out with use of the TMMP of Animalu in [50]. The **Table 10** provides radiuses of the first four coordination spheres and values of radial and tangential force constants for *Mg*, *Zr*, and *Ti*. The table shows the following characteristics: force constants, corresponding to the first

Table 10
Calculated values of radial α_i and tangential β_i force constants Mg , Zr и Ti , (10^{-3} N/m).

Number sphere i	Mg		Ti		Zr	
	α_i	β_i	α_i	β_i	α_i	β_i
1	14100	12	29500	2000	24200	1100
2	10400	10	12300	1200	11700	700
3	1200	-330	2400	-720	3700	-1300
4	-520	-60	700	-190	1200	430

and second coordination spheres, they have similar values for each of the elements, which is the result of close values of radiuses of these spheres. Radial force constant for each of the coordination spheres is greater than tangential constant.

Elastic constants for Mg , Zr and Ti , calculated above by the given method in [50] when comparing with experimental values [51-53], are given in **Table 11**. Elastic constants for magnesium, calculated by the method, using functions of electronic density distribution [47], are also given. The conclusion is drawn in [50] that calculation of elastic constants of Mg by method of a model potential gives the same satisfactory agreement with experiment as well as the calculation with use of function of an electronic density distribution [47]. A satisfactory similarity of the calculated values of elastic constants with the experimental data is also received for Ti and Zr . At the same time, values of elastic constants of C_{12} , C_{13} , and C_{33} are closer to the experiment. Discrepancy for elastic constants C_{11} and C_{44} does not exceed

Table 11
Elastic constants Mg , Zr и Ti , (10^{10} N/m²).

	Reference	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
Mg	[50]	7.1	3.2	3.4	8.4	1.7
	[47]	5.9	2.6	2.1	6.2	1.6
	Exp.[53]	8.3	3.2	1.9	9.7	1.8
Ti	Exp.[51]	6.3	2.5	2.1	6.6	1.8
	[50]	21.7	8.1	7.5	20.6	5.9
Zr	Exp.[51]	16.2	9.2	6.9	18.1	4.6
	[50]	17.5	6.3	6.1	19.8	2.5
	Exp.[51]	14.4	7.2	6.5	16.5	3.2
	Exp.[52]	14.3	7.3	6.5	16.5	3.2

15%. It is noted that this discrepancy may be due to imitation by only four coordination spheres.

10. CALCULATION OF FORCE AND ELASTIC CONSTANTS FOR ALLOYS BY THE PSEUDOPOTENTIAL METHOD

Calculation method of force and elastic constants for FCC alloys by the pseudopotential method in the De Launay's model is proposed in [13, 24], where the TMMP of Animalu [19, 20] is used for alloys $Co_{0.92}Fe_{0.08}$ and $Ni_{0.55}Pd_{0.45}$. Thus, radial and tangential force constants of an alloy were calculated by method of an averaging of force constant components. With use of such calculated force constants, phonon spectrums, functions of phonon states' density, temperature dependences of a thermal capacity and Debye temperature of alloys $Co_{0.92}Fe_{0.08}$ and $Ni_{0.55}Pd_{0.45}$ were created. Elastic constants of $Co_{0.92}Fe_{0.08}$ and $Ni_{0.55}Pd_{0.45}$ alloys, calculated in [13, 24], are given in **Table 12**. Values of elastic constants of the $Co_{0.92}Fe_{0.08}$ alloy, calculated with use of the Born-Karman's force constants in the first four coordination spheres, which are taken from the experimentally measured phonon spectrum [54], are also provided there. Value of an elastic constant of C_{11} , calculated in [13], is close to the result [54], and the satisfactory consent with results is observed for other two constants [54].

An attempt to spread the methods [13, 24] on calculations of elastic constants of some multicomponent alloys, the results of which are shown in **Table 13** when comparing to experimental data, was made in [55]. Having surveyed the table data, it can be concluded that

Table 12
Elastic constants of alloys $Co_{0.92}Fe_{0.08}$ and $Ni_{0.55}Pd_{0.45}$ (10^{10} N/m²).

Alloy	Reference	C_{11}	C_{12}	C_{44}
$Co_{0.92}Fe_{0.08}$	[13]	21.83	16.70	8.30
	Exp.[54]	22.1	14.7	12.4
$Ni_{0.55}Pd_{0.45}$	[13]	22.45	19.43	7.48

Table 13
Calculations results of the elastic constants of some FCC alloys with MPPM of Animalu (10¹⁰ N/m²).

Alloy	Reference	C ₁₁	C ₁₂	C ₄₄
Cu _{0.75} Zn _{0.25}	[55]	14.7	13.0	5.0
	Exp. [56]	14.5	10.7	7.1
Ni _{0.804} Cr _{0.196}	[55]	24.5	19.1	8.8
	Exp. [57]	24.7	15.4	12.2
Ni _{0.502} Fe _{0.498}	[55]	20.7	14.1	7.4
	Exp. [58]	20.5	14.6	10.8
Ni _{0.738} Fe _{0.262}	[55]	22.4	16.3	7.8
	Exp. [59]	23.0	14.4	11.9
Ni _{0.892} Fe _{0.108}	[55]	23.0	18.1	8.6
	Exp. [60]	25.5	15.3	13.0
Fe _{0.76} Cr _{0.12} Ni _{0.12}	[55]	22.9	15.0	8.2
	Exp. [61]	23.3	16.3	12.3
Fe _{0.705} Cr _{0.175} Ni _{0.120}	[55]	22.2	15.2	8.2
	Exp. [62]	21.6	14.4	12.9
Fe _{0.685} Cr _{0.145} Ni _{0.145} Mo _{0.025}	[55]	22.6	12.9	7.3
	Exp. [57]	20.4	13.4	12.9

the calculation results are in good agreement with experimental data [56-63].

Calculations of force and elastic constant for BCC alloys of Fe-Re 3, 5 and 7 at.%Re with use of the TMMP of Animalu by formulas (35)-(38) are carried out in [63], which results are shown in Table 14. Force constants of these alloys were averaged from radial and tangential force constant of Fe and Re, which are given in Tab. 6. Thus, force constants of Re were calculated in an iron's matrix. The calculated values of elastic constant for alloys Fe 3, 5, 7 at.%Re are successfully applied to process an intensity of diffusion dispersion of X-rays of these alloys and calculations of short-range order parameters and ordering energy [63].

Table 14
Elastic constants of alloys Fe 3, 5, 7 at.%Re [63].

Alloy	Elastic constants (10 ¹⁰ N/m ²)		
	C ₁₁	C ₁₂	C ₄₄
Fe 3at.%Re	24.9	15.2	12.8
Fe 5at.%Re	24.1	14.7	12.2
Fe 7at.%Re	23.3	14.1	12.1

Table 15
Elastic constants (10¹⁰ N/m²) alloys of Pd_{1-x}Fe_x at T = 300K. Values in parentheses indicate the divergence of the calculated from the experimental values in percentage.

	x = 0.04		x = 0.10		x = 0.28	
	calc.[27]	exp.[64]	calc.[27]	exp.[64]	calc.[27]	exp.[65]
C ₁₁	17.16(-25)	23.0	17.24(-25)	22.9	17.91(+28)	14.0±0.2
C ₁₂	12.76(-17)	15.3	12.92(-22)	16.5	13.8(+3)	13.4±0.2
C ₄₄	10.15(+30)	7.8	10.04(+14)	8.6	9.92(+24)	8.00±0.02

Elastic constants of alloys Pd_{1-x}Fe_x (x = 0.04, 0.1, 0.28) to FCC structure are calculated by the G. Squires's formulas (44) in [27]. Thus, the alloy's force constants were calculated by an averaging of force constant components based on concentration. The calculated radial and tangential force constants of Pd in [27] are shown in Table 5, and for γ-Fe – in Table 7. These values were calculated by the pseudopotential method, taking into account contributions of s and d electrons, and their reliability were checked by calculations of phonon spectrum and elastic constants of corresponding metals. The calculated values of elastic constants for alloys Pd_{1-x}Fe_x are given in Table 15 when comparing with experimental data [64, 65], and the author [27] concluded that calculation of contributions for s and d electrons in the iron-based alloys is competent.

11. CONCLUSION

Review of two calculation methods for dynamics of a crystal lattice is provided in this work: the Born-Karman and De Launay's models. These models are different in definitions of atomic interaction force constants. In the Born-Karman's model, force constants have a tensor appearance, but in the De Launay's model they are determined by first and second derivatives of pair atomic interaction potential, which are referred to as tangential and radial force constants. However, there is an interrelation between these two definitions that can be used when comparing results of the two calculation methods. So, the example of calculations of elastic constants for alkaline metals shows an

adequacy of the Squires's formulas (44), which involve the Born-Karman's force constants, and general formulas (47) to calculate elastic constants for *FCC* and *BCC* metals. Results of calculations of elastic constants for nickel and palladium, conducted by the formulas (30)-(32) of calculations of elastic constants for *FCC* metals, consistent with the results of calculations by the general formulas (47). Thus, we can conclude that the generalization of the formulas for calculating the elastic constants for *FCC* and *BCC* metals is competent.

Comparison of calculation results of force constants for particular metal using various types of model potential shows that sets of radial and tangential force constants generally differ, except for force constants in the first coordination sphere. This fact can be explained by the reason that an interaction between an atom in the reference point and its nearest atom is the strongest. The proof of reliability of theoretically certain force constants is a calculation with use of them of a phonon spectrum of this metal and comparison with an experimental spectrum. It is possible to estimate elastic constants of a metal and to compare with their experimental values from the calculated phonon spectrum in a long-wave approximation. Generally, it is possible to note that the pseudopotential method allows to estimate force and elastic constants of metals and alloys.

Based on the given results of calculations of elastic constants for cubic metals and alloys by the pseudopotential method, it is possible to conclude that the C_{11} value is almost always close to experimental value, and any of C_{12} and C_{44} considerably differs from experimental value. The reason for this can be explained, for example, by formulas (32) and (35), wherein the sum of elastic constants C_{12} and C_{44} are expressed in terms of linear combinations of force constants.

On the example of calculations of elastic constants for *Fe*, it is shown that the pseudopotential theory doesn't concede the theory of electronic state density functionality

in calculations of a lattice dynamics, and also provided information on force constants of atomic interaction.

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