Construction of primitive cells of the cubic syngony on the basis of the molecular acoustics method

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Abstract: Topicality of the present article is connected with introduction of new verifying condition, which is required for estimation of structures of cores of the "elementary" lattices of the body-centred cell and face-centred cell (these lattices were proposed in accordance with the Bravais theory), on the basis of theoretical calculations of the ultrasonic velocities, which are directed along the edges of the selected cells and which are verified with the help of the experimental data that were obtained in accordance with the molecular analysis method. The purpose of the present investigation was as follows: to carry out evaluation of the core structures of the elementary and primitive cells of the body-centred and face-centred cell of the crystal lattice of the cubic syngony (for alpha iron and cuprum) in respect of their conformity with methods of the molecular acoustics. The method of the present investigation is based on comparison of values of the ultrasonic velocities (longitudinal velocity, transversal velocity, and velocity within the rod), which were calculated on the basis of the relevant theory and which are transmitted over edges of the primitive cell that is constructed (for alpha iron and cuprum), with the values of these velocities of the ultrasound, which were obtained experimentally with the help of the molecular acoustics method for these materials. Introduction of the additional criterion (requirement) in respect of selection of the least cell on the basis of the molecular analysis has made it possible to draw the conclusion that cores of the "elementary" cells of the body-centred and face-centred crystal lattices, which are determined in accordance with the Bravais theory and which are assumed as the basis of the analysis with the help of the analytic geometry method, are inconsistent with actually existing mechanism of transmission of the ultrasound over the interatomic bonds (edges of the cell). In addition, this conclusion has made it possible to reveal new type (that is, a new syngony), which is the basis of the core structure of these "elementary" cells. The theoretically calculated ultrasonic velocities, which are directed along the edges of the primitive cell of the new type (for alpha iron and for cuprum), have been coincident with high accuracy with the values of the longitudinal and transversal sound velocity, as well as with the sound velocity within the rod, which were experimentally established with the help of the molecular acoustics method.

Keywords: interatomic distance, parameters of the crystal lattice, core of the cell, longitudinal velocity, transversal velocity, frequency of vibrations, monoatomic two-dimensional planes.

1. Introduction

Physical and mechanical parameters (PMP), such as velocity of the ultrasound in the relevant material or mechanical strength characteristics (Young's modulus of elasticity, modulus of transverse elasticity G, and other parameters) are usually determined in the course of relevant experiments. These characteristics are always connected with the structure of the relevant material, that is with the relevant parameters of the elementary cell [1-2]. However, ambiguity of the criteria, which are usually applied and which determine types of various crystal lattices (see Figure 1), desire for introduction of maximum quantity of straight angles, which simplify description of elementary cells, as well as different quantities of atoms, which are contained within the unit volume of "elementary" cells, violate relevant principle of unity in respect of...
selection of the cell structures in accordance with the Bravais theory. In addition, this theory does not envisage any possibilities of existence of the monoatomic two-dimensional materials [3], which were found during previous years.

The main attention in the present article was paid to the cubic syngony (see Figure 2), because of majority of materials, which are used in the metal goods industry, are always characterised by this kind of crystal lattices. It is well known that geometrical theory of development of the crystal structure was proposed by Bravais in 1849 [4], as well as that this theory is utilised (up to the present time) for development of mathematical models in the course of investigation of structure of various materials with the help of the following methods: method of deformation, method of the X-ray analysis of crystal structure, as well as with the help of the molecular acoustics method.

| Syngony          | Type of the crystal lattice | Characteristic of the crystal lattice |
|------------------|-----------------------------|--------------------------------------|
| Triclinic lattice | Primitive crystal lattice    | \(a = b = c\)                         |
|                  | Ortho-centred lattice       | \(a = \beta = \gamma \neq 90^\circ\) |
| Monoclinic lattice|                            |                                      |
|                  |                            | \(a = b = c\)                         |
|                  |                            | \(a = \beta = \gamma \neq 90^\circ\) |
| Rhombic lattice  |                            |                                      |
|                  |                            | \(a = b = c\)                         |
|                  |                            | \(\alpha - \gamma = 90^\circ, \beta = 90^\circ\) |
| Trigonal (rhombohedral lattice) | | \(a = b = c\) |
|                  |                            | \(\alpha - \beta - \gamma \neq 90^\circ\) |
| Tetragonal lattice |                            | \(a = b = c\)                         |
|                  |                            | \(\alpha = \beta = \gamma \neq 90^\circ\) |
| Hexagonal lattice |                            | \(a = b = c\)                         |
|                  |                            | \(\alpha = \beta = \gamma \neq 120^\circ\) |
| Cubic lattice    |                            | \(a = b = c\)                         |
|                  |                            | \(\alpha = \beta = \gamma \neq 90^\circ\) |

**Figure 1.** Types of the crystal lattice depending on the syngony

2. Materials and Methods

In the course of analysis of all the syngonies, which are presented in the Figure 1, in accordance with the Bravais theory, it is necessary to pay attention to the fact that volumes of the primitive cells (with the tetragonal, rhombic, rhombohedral, monoclinic, triclinic and cubic syngonies) are only created by means of interaction of the atoms, which are only situated in two neighbouring parallel planes. It is possible that, in the course of introduction of such determination Bravais supposed existence of certain monoatomic two-dimensional materials. However, Mr. Bravais did not introduce any determination of the monoatomic two-dimensional materials. Therefore, taking into consideration relevant classification of types of the crystal lattices, which are presented in the Figure 1, it is possible to demonstrate that there exist certain cores of crystal lattices, structure of cells of which is created in three atomic planes.

So, for example, crystal lattices in the cubic syngony are created both by two atomic planes \(\alpha\) and \(\beta\) (see Figure 2a), and three atomic planes \(\alpha\), \(\beta\), and \(\gamma\) (see Figure 2 b-c), which are revealed in the course of analysis of the "elementary" cells of the BCC-lattice (body-centred cubic lattice) and the FCC-lattice (face-centred cubic lattice) by means of assignment of the "primitive" cell, within which the cell volume is created at the expense of the interatomic interaction of atoms, which are situated in two neighbouring parallel planes (see Figure 3 a-b) [5].
Therefore, a primitive cell is usually presented as the minimum volume of the crystal. Translations of this crystal volume in three dimensions (parallel translations) make it possible to construct the three-dimensional crystal lattice of the entire volume of the relevant material. Such elementary cell is usually characterised by the fact that it must comply with the symmetry elements of the final volume, as well as with the properties of the relevant crystal [6].

In his theory, Mr. Bravais has formulated three rules for selection of elementary cells:
1. Symmetry of the elementary cell must comply with the symmetry of the relevant crystal.
2. The elementary cell must have maximum quantity of equal edges and equal angles.
3. Subject to fulfilment of these two rules, the elementary cell must have the least volume.

Let us introduce the additional condition in respect of selection of elementary cells of crystal lattices of various materials (because of the fact that elementary cell must comply with the physical and mechanical parameters of the crystal) with the help of the following statement:
4. Longitudinal velocity and transversal velocity of the ultrasound transmission within the material volume, which are determined in the course of relevant experiments, must comply with the theoretically calculated sound velocities, which propagate along the edges of the elementary cell that was constructed (that is, selected), thus confirming conditions of actual existence of such elementary cell. Therefore, in order to ensure strict assignment of the elementary (primitive) cell in this article, we will utilise the molecular acoustics method, which ensures possibility to compare velocities of transmission of the sound (ultrasonic) waves in the material [7], provided that these velocities were obtained in accordance with relevant experiments, as well as with the help of theoretical calculations.

Taking into consideration the fact that longitudinal velocity of the ultrasound propagates over the interatomic bonds within the monoatomic planes along the edge length, which is constructed (that is, selected) for the elementary (primitive) cell, as well as taking into consideration the fact that the wave length is limited by any maximum value, which (in accordance with results of article [8]) is approximately equal to double radius of atoms, then it is possible to present the wave length ($\lambda$) with the help of the following expression:
$$\lambda = 2 \cdot R$$

where $R$ is the interatomic distance, which is equal to the edge length within the plane, while $\omega$ denotes the natural frequency of vibration of atoms in the planes, which create volume of the elementary (primitive) cell of the relevant material.

We have to take into consideration the fact that natural frequency of vibration of atoms within the elementary cell is limited by certain maximum frequency $\omega_{\text{max}}$ [9] that has the same value for all the atoms, which create volume of the elementary (primitive) cell [10]. At the same time, it is assumed that lengths of edges within the cubic primitive cells are the same ($a = \lambda$). Therefore, in accordance with equation (2), values
of the longitudinal and transversal velocities of ultrasound must have the same values (this fact can be confirmed in the course of investigation of the polonium, which has the same structure: the cubic crystal lattice).

However, it is known [11-12] that longitudinal and transversal sound velocities for the iron (BCC-lattice elementary cell) and copper (FCC-lattice elementary cell), which were determined in the course of relevant experiments with the help of the method of molecular acoustics, are different. It is only possible to explain this discrepancy taking into consideration the fact that all volumes of the primitive cells are created at the expense of the interatomic interactions of the atoms, which are situated in two neighbouring monoatomic parallel planes. At the same time, in the elementary crystal lattice, within which the intermediate plane \( \beta \) exists (see Figure 4), the prohibition occurs in respect of interatomic interactions of the atoms between planes \( \alpha \) and \( \gamma \). It is possible that in this case the ultrasound velocity can distribute over the interatomic bonds at the level of minimum resistance. Therefore, let us introduce relevant prohibition in respect of interatomic interaction of atoms through the intermediate plane in order to ensure further theoretical analysis.

Now let us calculate velocity of the ultrasonic wave for iron (Fe) and copper (Cu) on the basis of the introduced condition. From the very beginning, it is necessary to do the following: we have to construct the "elementary" cell of iron with the help of the atoms, which are situated in three parallel planes \( \alpha \), \( \beta \), and \( \gamma \) (see Figure 4).

![Figure 4](image)

*Figure 4.* "Core" of the elementary body-centred cubic cell of the crystal lattice of iron. This core is created with the help of the atoms, which have sequential numbers from 0 to 8 and which are situated within the monoatomic two-dimensional parallel planes \( \alpha \), \( \beta \), and \( \gamma \).

Having assumed that energy of the ultrasound has already achieved the atom No. 0, let us analyse further transmission of energy over the bonds between the atoms, which create the "core" of the elementary cell of the BCC crystal lattice of iron (see Figure 4). This "core" is created with the help of two "primitive" cells, type of which is described in article [5]. The first cell is created with the help of the atoms, which have sequential numbers 1, 2, 3, and 4 and which are situated within the plane \( \alpha \), as well as with the help of the atoms, which have sequential numbers 0, 12, 13, and 14 and which are situated within the neighbouring parallel plane \( \beta \). The second cell is created with the help of the atoms, which have sequential numbers 11, 10, 9, and 0 and which are situated within the plane \( \beta \), as well as with the help of the atoms, which have sequential numbers 5, 6, 7, 8 and which are situated within the neighbouring parallel plane \( \gamma \). In this case, these primitive cells comply with the relevant criteria for selection of cells. These criteria were proposed in accordance with the Bravais theory and they were described above already. Due to introduction of the restriction in respect of the interatomic interactions through a plane, there are no transmissions of the ultrasonic waves over the following edges of the core of the "elementary" cell: L1-8, L2-7, L3-6, and L4-5. The longitudinal velocity of ultrasound exists within the monoatomic two-dimensional planes \( \alpha \), \( \beta \), and \( \gamma \) over the edges (interatomic bonds) of primitive cells of the following types: L1-2, L9-11, and L7-8. With the help of the experimentally established value of the longitudinal velocity of ultrasound in iron (in accordance with the data of article [13]), which is equal to 5.940 m/s, as well as with the help of the edge length L1-8, which is equal to \( 3 \times 10^{-10} \) m (in accordance with article [10]; this fact is connected with introduction of the unified principle of the interatomic interaction for the cell volume), let us calculate frequency of vibration of atoms in accordance with the following formula:

\[
\omega_{\text{max}} = \frac{v_{\text{longitudinal}}}{\lambda},
\]

\[
\omega_{\text{max}} = 5.940 \text{ (m/s)} / 3 \times 10^{-10} \text{ (m)} = 1.98 \times 10^{13} \text{ Hz}. \quad (3, 4)
\]
3. Results and Discussion

In order to calculate transversal velocity of ultrasound within the core of the "elementary" cell of the BCC crystal lattice of iron, let us determine the length of the interatomic bond \( L \ 1-0 \) with the help of the length of the interatomic interaction \( L \ 1-2 \) of the atoms, which are situated within the plane \( \alpha \) (length of the interatomic interaction in any of three monoatomic planes \( \alpha, \beta \) or \( \gamma \) has the constant value: \( L \ 1-2 = L \ 9-11 = L \ 8-7 \)). Due to the fact that the central atom (which has sequential number No. 0 and which is assumed as the atom, through which sound is transmitted) is situated in the middle of the space diagonal, then (with the help of the theorem of Pythagoras) it is possible to calculate length of the interatomic interaction of the atoms, which are situated within the plane \( \beta \), with the atoms, which are situated in the planes \( \alpha \) and \( \gamma \):

\[
L \ 1-0 = L \ 0-6 = L \ 1-2 \times (\sqrt{3}) / 2, \tag{5}
\]

\[
L \ 1-0 = 3 \times 10^{-10} \times (\sqrt{3}) / 2 = 2.598 \times 10^{-10} \text{ m}, \tag{6}
\]

The time \( t \) (in seconds) of transmission of the ultrasound wave over the length of the interatomic bond \( L \ 1-0 \) (taking into consideration the fact that frequency of vibration of atoms for the core of the elementary cell has the constant value) will be equal to:

\[
t \ 1-0 = 1 / \omega_{\text{max}} = 1 / 1.98 \times 10^{13} \text{ Hz} = 0.505 \times 10^{-13} \text{ seconds}, \tag{7}
\]

The theoretical value of velocity of the ultrasound transmission between the monoatomic planes \( \alpha \) – \( \beta \) and \( \beta \) – \( \gamma \) will have the following value:

\[
u \ 1-0 = L \ 1-0 / t \ 1-0 = 2.598 \times 10^{-10} \text{ m} / 0.505 \times 10^{-13} \text{ s} = 5.144 \times 10^{3} \text{ m/s}, \tag{8}
\]

Then, it is possible to calculate the theoretical value of velocity of the transversal wave in the following manner:

\[
u_{\text{transversal}} = L \ 7-2 / (t \ 1-0 + t \ 0-6), \tag{9}
\]

where \( L \ 7-2 \) denotes the "fictitious" interatomic bond between planes \( \alpha \) and \( \gamma \).\n
\[
\tau \ 1-0 = \tau \ 0-6 = 1 / \omega_{\text{max}}. \tag{10}
\]

In addition, equation (9) can be presented in the following form:

\[
u_{\text{transversal}} = L \ 7-2 / ((1/\omega_{\alpha}) + (1/\omega_{\gamma})) = L \ 7-2 \times \omega_{\text{max}} / 2. \tag{11}
\]

If we will substitute value of the "fictitious" length of the interatomic bond (in accordance with the condition, which we have introduced, this interatomic bond does not exist), which is equal to \( 3 \times 10^{-10} \text{ m} \), and if we will substitute value of frequency of vibration of atoms in the planes, which create core of the elementary cell (this frequency is equal to \( 1.98 \times 10^{13} \text{ Hz} \)), into equation (11), then we will calculate the following theoretical value of transversal velocity of ultrasound:

\[
u_{\text{transversal}} = 3 \times 10^{-10} \text{ m} \times 1.98 \times 10^{13} \text{ Hz} / 2 = 2.973 \times 10^{3} \text{ m/s} = 2.940 \text{ m/s}, \tag{12}
\]

It is well known that value of the transversal velocity of ultrasound, which was obtained in accordance with relevant experiments with the help of the molecular acoustics method, has the value which is equal to \( \nu_{\text{transversal}} = 3.100 \pm 100 \text{ m/s} \) in accordance with the data of article [13]. In fact, the transversal velocity of ultrasound, which was calculated on the basis of new model of construction of the core of the "elementary" cell (taking into consideration the introduced restriction in respect of the interatomic interactions of atoms through the intermediate plane), has coincided with the lower boundary of the experimentally established value of transversal velocity of ultrasound in iron.

Theoretical value of the ultrasound velocity in the equation (8) \( \nu \ 1-0 = 5.144 \times 10^{3} \text{ m/s} \). This value describes transmission of the ultrasound over the face of the primitive cell between two monoatomic parallel planes is in line with the ultrasound velocity within the rod of iron. The experimentally established value of the ultrasound velocity (which was calculated with the help of the method of molecular acoustics) within the iron rod has the following value: \( \nu_{\text{transversal}} = 5.170 \text{ m/s} \) [13]. Values of these velocities coincide with each other in accordance with the following percentage:

\[
\% = [5.148/5.170] \times 100\% = 99.574 \%, \tag{13}
\]

Coincidence of the ultrasound velocity along the edge of the primitive cell between planes and velocity of ultrasound within the rod can be caused by the fact that the rod has the strictly assigned ratio between the length and diameter.
Coincidence of the theoretically calculated values of the longitudinal velocity, transversal velocity and velocity of ultrasound within the rod was obtained due to taking into consideration the single frequency $\omega_{\text{max}}$ = $\omega_{\text{dem}}$ of vibration of all atoms within the core of the "elementary" cell of iron in respect of all interatomic bonds (both within parallel atomic planes and within the interatomic bonds, which connect neighbouring planes). All theoretical calculations of the ultrasound velocity can be presented with the help of the single equation, which was proposed in article [10] and which is presented below:

$$\nu = \frac{L \times \omega}{n},$$  \hspace{1cm} (14)

where $L$ denotes length of the interatomic distance, which is expressed through the length of the interatomic bond of atoms, which are situated within the plane.

$\omega$ denotes frequency of vibration of atoms within the core of the "elementary" (primitive) cell of the crystal lattice of iron.

$n$ denotes quantity of the interatomic interactions, which are used for transmission of the ultrasound to different planes within the core of the elementary (primitive) cell of the crystal lattice.

**Figure 5.** Core of the "elementary" of the face-centred cubic crystal lattice that is created with the help of the atoms, which are situated in three parallel planes $\alpha$, $\beta$, and $\gamma$.

Introduction of the new verifying condition in the course of selection of the elementary cell, as well transmission of the ultrasound wave over edges of the cell, which is constructed, have demonstrated that the "elementary" cell of the BCC crystal lattice (this "elementary" cell was proposed in accordance with the Bravais theory) does not exist, because of the interatomic bond between planes $\alpha$ and $\gamma$ does not exist. In this case, relevant cell (Figure 3a), which is considered as the "primitive" cell and which is the basis of structure of the "elementary" cell, describes actual process of transmission of the ultrasound over edges of the present cell. Such "primitive" cell complies with conditions of construction, which are used for the rest types of primitive cells in accordance with the Bravais theory, in accordance with which the cell volume is only created with the help of the atoms, which are situated in two neighbouring parallel monoatomic planes $\alpha$ and $\beta$.

Let us perform similar theoretical analysis of structure of the "elementary" cell of copper, which has the FCC crystal lattice and which belongs to the cubic syngony as well. In order to do that, we will construct the core of the "elementary" cell of copper with the help of the atoms, which are situated in three parallel planes $\alpha$, $\beta$, and $\gamma$ (see Figure 5).

Atoms with subsequent numbers 1-14 (see Figure 5) are in correspondence with the entire core of the "elementary" face-centred cell, which is created with the help of atoms of four primitive cells [5] (see Figure 6).
Let us calculate frequency of vibration of atoms in the planes $\alpha$, $\beta$, and $\gamma$ with the help of values of the longitudinal velocity of ultrasound, which were determined experimentally with the help of the molecular acoustics method. Value of this longitudinal velocity is presented in article [13] as $v_{\text{long}} = 4,700$ m/s. Let us assume (on the basis of condition of the unified principle of the interatomic interaction) that value of parameter of the edge of the "elementary" cell of copper is equal to $L_{1-2} = 3.65 \times 10^{-10}$ m. This value was determined in the course of theoretical calculation, which is presented in article [10]. As concerns the core of the "elementary" cell of the FCC crystal lattice, the edge length of the primitive cell $L_{3-4}$ does not comply with the edge length $L_{1-2}$ (L 3-2) of the core of the elementary cell. This situation is observed within the primitive cell of the BCC crystal lattice. Because of the fact of introduction of the fourth point in respect of transmission of the ultrasound over edges of primitive cells, let us assume that longitudinal velocity of ultrasound will propagate along the edge length $L_{3-4}$. Let us present the edge length of the primitive cell through the edge length of the "elementary" cell $L_{1-2}$ as follows:

$$L_{3-4} = L_{1-2} \times (\sqrt{2}/2) = 3.65 \times 10^{-10} \times 0.707 = 2.58 \times 10^{-10} \text{m},$$

(15)

Let us calculate value of frequency $\omega_{\text{Cu}}$ for the atoms, which create volume of the primitive cell:

$$\omega_{\text{Cu}} = \frac{v_{\text{long}} \text{Cu}}{L_{3-4}} = \frac{4.700 \text{m/s}}{2.58 \times 10^{-10} \text{m}} = 1.821 \times 10^{13} \text{Hz},$$

(16)

We will calculate velocity of the ultrasound transmission along the length of the edge, which connects planes $\alpha$ and $\beta$ of the primitive cell $L_{3-13}$, in the following manner:

$$v_{3-13} = L_{3-13} \times \omega_{\text{Cu}},$$

(17)

In order to perform this calculation, we will present length of the space edge of the primitive cell $L_{3-13}$ with the help of the length of the interatomic interaction of atoms within the core of the FCC crystal lattice $L_{3-2}$ and $L_{1-2}$ as follows:

$$L_{3-13} = L_{1-2} \times (\sqrt{2}/2) = 2.58 \times 10^{-10} \text{m},$$

(18)

If we will substitute value of length of the space edge of the primitive cell $L_{3-13}$ from equation (18) into equation (17), then we will calculate the following value of velocity of the ultrasound transmission:

$$v_{3-13} = 2.58 \times 10^{-10} \times 1.821 \times 10^{13} \text{Hz} = 4.700 \text{m/s},$$

(19)

This theoretically calculated value of velocity of the ultrasound transmission along the edge, which connects atoms in two neighbouring parallel planes, has coincided with the value of longitudinal velocity of ultrasound within the FCC crystal lattice of copper. At the same time, the experimentally established value of the ultrasound velocity within the copper rod is equal to 3,700 m/s. Taking into consideration the fact that velocity of ultrasound within the iron rod has been complied with the theoretically calculated value of the ultrasound velocity along the edge (that is over the interatomic interaction of planes $\alpha$ and $\beta$ of the primitive cell of the BCC crystal lattice), then it is possible to expect that mechanism of the ultrasound transmission velocity within the rod (in accordance with the principle of uniformity) within the primitive cell of the FCC crystal lattice of copper must be the same or similar. Therefore, it is not expedient to perform further analysis of such primitive cell (see Figure 6).

This is the reason why we will introduce the additional condition for selection of primitive cells: maximum length of the primitive cell edge must coincide with the maximum length of the interatomic
interaction of atoms within the monoatomic plane. So, let us construct new primitive cell, which creates the core of the "elementary" cell of the FCC crystal lattice of copper (see Figure 7).

Fig. 7. Structure of the primitive cell of the FCC crystal lattice that is created with the help of the atoms, which are situated in two parallel planes and which comply with the introduced condition in respect of the maximum length of the interatomic bond within the plane.

Fig. 8. Core of the "elementary" cell of the FCC crystal lattice. This core is created with the help of four new primitive cells

Figure 7 presents structure of the primitive cell of the FCC crystal lattice. This structure is created with the help of the atoms that are situated in two parallel planes and this structure complies with the introduced condition in respect of the maximum length of the interatomic bond within the plane.

Let us perform construction of the core of the "elementary" cell of the FCC crystal lattice with the help of the atoms, which are situated in three planes α, β, and γ, taking into consideration structure of such new primitive cell (see Figure 8).

Now let us calculate frequency of vibration of atoms ωCu in the planes α, β, and γ for the volume of such new primitive cell. In accordance with the results of article [10], maximum edge length of the primitive cell is equal to L 1-2 = 3.65×10⁻¹⁰ m. This length complies with the velocity of ultrasound, which is equal to 4.700 m/s (see article [9]) and which was determined experimentally with the help of the method of molecular acoustics. Therefore, frequency of vibration of atoms will have the value, which is equal to:

$$\omega_{Cu} = 4.700 \text{ m/s} / 3.65\times10^{-10} \text{ m} = 1.287\times10^{13} \text{ Hz}$$

Taking into consideration the fact that value of frequency of vibration of atoms, which was determined in the equation (20) in the same manner for all atoms (both within the primitive cells of the FCC lattice, and within the core of the "elementary" cell of the FCC crystal lattice of copper), let us calculate velocity of ultrasound along the edge that determines interatomic interaction of the atoms, which are situated in the planes α and β, L1-7 (see Figure 7):

$$v_{1-7} = L_{1-7} \times \omega_{Cu}$$

Let us present value of the space edge length L1-7 with the help of the edge length L1-2 in the following manner:

$$L_{1-7} = L_{3-2} \times (\sqrt{2} / 2) = 2.58\times10^{-10} \text{ m}$$

Therefore, if we will substitute this value into (21), then we will calculate value of the ultrasound velocity between the atoms, which are situated within the neighbouring parallel planes α and β. That is, this value corresponds to the edge of the primitive cell:
\[ v_{1-7} = 2.58 \times 10^{-10} \text{ m} \times 1.287 \times 10^{13} \text{ Hz} = 3.320 \times 10^5 \text{ m/s}, \]

This value of the ultrasound velocity, which was theoretically calculated on the basis of the space diagonal and on the basis of the primitive cell edge, practically corresponds to the velocity of ultrasound within the copper rod. Difference of the theoretically calculated value of the sound velocity within the rod from the experimentally established value of the ultrasound velocity within the rod (which was determined with the help of the method of molecular acoustics), \( u_{\text{act}} = 3.700 \text{ m/s} \), is equal to:

\[ \% = \left( \frac{3700 - 3328}{3700} \right) \times 100\% = 10\%, \]

This error (10\% only) is the allowable deviation due to the error in determination of parameters of the interatomic distance with the help of the method of the X-ray analysis of crystal structure (due to vibration of an atom near the equilibrium position [10]).

We will use the following formula in order to calculate theoretical value of the transversal velocity of ultrasound within the core of the "elementary" cell of the FCC crystal lattice of copper:

\[ v_{2-11} = L \times 2-11 \times \omega_{\text{Cu}} \times (1/n), \]

It is necessary to point out that (in accordance with the accepted restriction in respect of the interatomic interaction through the plane) length L2-11 is the "fictitious" length. Therefore, quantity of the interatomic interactions \( n \), which are required for transmission of ultrasound from the monoatomic plane \( a \) into the monoatomic plane \( \gamma \), will have the value, which will be equal to 2 (two). Then, respectively, the transversal velocity will have the value, which is equal to:

\[ u_{\text{transversal Cu}} = 3.62 \times 10^{-10} \text{ m} \times 1.298 \times 10^{13} \text{ Hz} \times (1/2) = 2.349 \times 10^5 \text{ m/s}, \]

This theoretically calculated value of the transversal velocity in copper \( (u_{\text{transversal Cu}} = 2.349 \text{ m/s}) \) differs from the experimental value of the transversal velocity 2.260 m/s (which was determined with the help of the method of molecular acoustics) by 3.9\% only. Therefore, new structure of the primitive cell of the FCC crystal lattice complies with the condition of the ultrasound transmission over edges of the cell, that is, it describes the actually existing interatomic bonds of atoms, which create the entire volume of the constructed cell. Therefore, (in the same manner, as it was in the previous situation with the "elementary" cell of the BCC crystal lattice) it is possible to draw the conclusion that the FCC "elementary cell", which was described in accordance with the Bravais theory as the cube, does not exist.

![Figure 9. Structures of such "primitive" cells](image)

Both structures of primitive cells of the BCC-lattice (Figure 2a) and the FCC-lattice (Figure 7) comply with the main principle, which was described in accordance with the Bravais theory. This principle was
described in the following manner: volume of the elementary cell is created with the help of the interatomic interaction of the atoms, which are situated in two neighbouring parallel monoatomic planes. In the course of thorough analysis of the structure of such "primitive" cells (see Figure 9 a-b), it is possible to determine the main characteristic of such primitive cells through the lengths of edges and relevant angles:

1. For the BCC-cell (Figure 9a) lengths of the edges \(a = b \neq c\), angles \(\angle \alpha^o = \angle \beta^o \neq \angle \gamma^o\);

2. For the FCC-cell (Figure 9b) lengths of the edges \(a \neq b = c\), angles \(\angle \alpha^o = \angle \beta^o \neq \angle \gamma^o\).

On the other hand (depending on the accepted names of sides of these primitive cells), it is possible to determine one common characteristic:

\[a = b \neq c, \angle \alpha^o = \angle \beta^o \neq \angle \gamma^o. \quad (27)\]

Development of the new type of the primitive cell confirms the idea of the Academician E. S. Fedorov (which he has formulated in article [14]) in respect of the fact that the process of selection of conditions of the symmetry is the most important factor for subsequent development of the interconnected theory for analysis of all aggregative processes, which occur within the crystal lattice. This theory was clearly demonstrated in this article with the help of selection (that is, construction) of various primitive cells as the core of the "elementary" cell of the BCC-lattice and the FCC crystal lattice.

4. Conclusion

In the course of the theoretical analysis, which was performed in this article, it was established that cores of the "elementary" cells of the body-centred and face-centred crystal lattices (these "elementary" cells were presented in accordance with the Bravais theory, they are used in the models for estimation of various physical and mechanical processes, which occur in the course of deformation, as well as they are the basis of the analytic geometry method) do not describe process of transmission of the ultrasound over the interatomic bonds, that is, over edges of the cell within the selected (that is, within the constructed) volume of the cell core. The discrepancy, which has appeared between structure of the core and actually existing interatomic bonds, has demonstrated that the interatomic bonds through the intermediate plane do not exist. It has also demonstrated that construction of the cubic syngony is implemented by taking into consideration the interatomic interactions of the atoms, which are only situated within two neighbouring parallel planes. This conclusion corresponds to the majority of types of lattices within the same theory of Bravais. Introduction of the additional condition in respect of structure of cells (that is, requirement in respect of transmission of the ultrasound over edges of the selected cell) has made it possible to determine new type of the primitive cell, which has the following characteristics of the crystal lattice: \(a = b \neq c, \angle \alpha^o = \angle \beta^o \neq \angle \gamma^o\). This type of the primitive cell is used for construction of cores of the BCC and the FCC "elementary" cells. The theoretically calculated values of the ultrasound velocity over faces of the new type of primitive cell (within the alpha iron and cuprum) have coincided with sufficiently high accuracy with the values of the longitudinal sound velocity, transversal sound velocity and with the sound velocity within the rod. These values were experimentally established with the help of the molecular acoustics method.

New approach to construction (selection) of the basics of structure of materials (that is, construction of the primitive cells, edges of which (lengths of the interatomic bonds) are in correspondence with the physical process of the ultrasound transmission) has provided the author of this article with possibility to carry out theoretical calculation of values of the Young's modulus of elasticity and G modulus of transverse elasticity with the help of parameters of primitive cells. Procedure of this theoretical calculation will be presented in the next article of the author, which will be published in future.

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