APERFEIÇOAMENTO DO MODELO DIATÔMICO DE INTERAÇÃO INTERATÓMICA DE FRENKEL PARA MELHORAR OS MÉTODOS DE CONTROLE DE QUALIDADE NÃO DESTRUTIVOS

REFINEMENT OF THE DIATOMIC MODEL OF THE INTERATOMIC INTERACTIONS OF FRENKEL FOR THE IMPROVEMENT OF METHODS OF NON-DESTRUCTIVE QUALITY CONTROL

УТОЧНЕНИЕ ДВУХАТОМНОЙ МОДЕЛИ МЕЖАТОМНОГО ВЗАИМОДЕЙСТВИЯ ФРЕНКЕЛЯ ДЛЯ УСОВЕРШЕНСТВОВАНИЯ МЕТОДОВ НЕРАЗРУШАЮЩЕГО КОНТРОЛЯ КАЧЕСТВА

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RESUMO

O objetivo do estudo é esclarecer o mecanismo de interação interatômica no modelo de Ya. I. Frenkel e associar este processo com a propagação de ultrassom na rede cristalina de metais, bem como com a velocidade de propagação de ultrassom em hastes de diferentes materiais tomados como amostras padrão para determinar o módulo de Young. Foi analisado o mecanismo de interação interatômica no modelo diatômico de Ya. I. Frenkel. Foi criado um modelo que ligava o processo de interação das camadas eletrônicas de átomos com a velocidade de propagação do som, levando em conta a estrutura da rede cristalina metálica. O novo modelo permite o cálculo teórico da velocidade de ultrassom em diferentes redes cristalinas de metais. Como resultado da pesquisa, verificou-se que os valores das velocidades de ultrassom calculados teoricamente coincidiam com uma precisão suficientemente alta com os valores obtidos experimentalmente de sua propagação, o que possibilita correlacionar o indicador de velocidade com as propriedades de resistência dos metais.

Palavras-chave: *distância interatômica, parâmetro de rede cristalina, velocidade longitudinal, velocidade transversal, velocidade do som na haste, frequência de oscilação de um átomo.*

ABSTRACT

The purpose of the study is to clarify the mechanism of interatomic interaction in the model of Ya.I. Frenkel and to link this process with the propagation of ultrasound in the crystal lattice of metals, as well as with the velocity of propagation of ultrasound in rods from different materials taken as standard samples for determining the Yung's modulus. An analysis of the mechanism of interatomic interaction in the diatomic model Ya.I. Frenkel is made. A model that linked the process of interaction of the electron shells of atoms with the speed of sound propagation was created, taking into account the structure of the metal crystal lattice. The new model allows the theoretical calculation of the ultrasound velocity in different crystal lattices of metals. In the result of the research, it was found that the theoretically calculated values of the ultrasound velocities with a sufficiently high accuracy coincided with the experimentally obtained values of its propagation, which makes it possible to correlate the rate indicator with the strength properties of metals.

Keywords: *interatomic distance, parameter of the crystal lattice, longitudinal velocity, transverse velocity, speed of sound in a rod, oscillation frequency of an atom.*

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АННОТАЦИЯ

Цель исследования – уточнить механизм межатомного взаимодействия в модели Я.И. Френкеля и связать данный процесс с распространением ультразвука в кристаллической решетке металлов, а также со скоростью распространения ультразвука в стержнях из разных материалов принятых в качестве стандартных образцов для определения модуля Юнга. Проведен анализ механизма межатомного взаимодействия в двухатомной модели Я.И. Френкеля. Создана модель, связавшая процесс взаимодействия электронных оболочек атомов со скоростью распространения звука, учитывающая строение кристаллической решетке металла. Новая модель позволяет проводить теоретический расчет скоростей ультразвука в разных кристаллических решетках металлов. В результате проведенных исследований было установлено, что теоретически рассчитанные значения скоростей ультразвука с достаточно высокой точностью совпали с экспериментально полученными значениями его распространения, что позволяет скоррелировать показатель скорости с прочностными свойствами металлов.

Ключевые слова: *межатомное расстояние, параметр кристаллической решетки, продольная скорость, поперечная скорость, скорость звука в стержне, частота колебания атома*.

INTRODUCTION

Increasing requirements to ensure the quality and reliability of new designs in conditions of real workloads require improvements in non-destructive testing methods to determine allowable loads based, for example, on the use of acoustic control of the ultrasound propagation velocity in finished products, and the results of which comparing with the ultrasound velocity propagation results obtained in determining the strength of control samples, by testing them till the complete destruction (Wright, 2017).

The difference of such method from the actual loading conditions is that under the destructive method, the external loading parameters of the control sample are regulated both by the size of the samples themselves and by the speed of their stretching, because only within these limits obtain the values of Yung's modulus for test materials, close to each other, which accept as the main characteristic of one or another material (Ashcroft and Mermin, 1977; Hamburg, 1997). In this, the model, that connecting the structure of the crystal lattice with the strength properties of metals, as well as with the speed of propagation of ultrasound in these metals do not exist (Kir, 1986; Maltseva *et al.*, 2007). Therefore, all calculations of the velocity of propagation of ultrasound are carried out on the basis of equations using the values of the Yung modulus.

MATERIALS AND METHODS

The relevance of the study of the structure of the crystal lattice of various metals is that all the physicomechanical parameters used in practice, for example, the speed of sound in the stem of the material or strength characteristics, which obtained experimentally and related with the composition of the structure of metal itself, determined by the parameters of the unit cell (Pearson, 2013; Zadiranov, 2008). In connection with different values of ultrasound velocities, obtained experimentally using the method of molecular acoustics, and the values obtained on the basis of equations using the Yung modulus, it is proposed, based on the refinement of the diatomic model of interatomic interaction Ya.I. Frenkel, create a theoretical model of the interatomic interaction in the crystal lattice to calculate the values of sound speeds through the parameters of the unit cell (Formalev *et al.*, 2017; Greshnov, 2007). What determines and the purpose of the research: clarification of the mechanism of interatomic interaction of the model Ya.I. Frenkel in metals, which allowed relating the process of ultrasound propagation in crystal lattices of metals with the sizes of these lattices.

The main research method was chosen theoretical analysis, which allowed to specify the model for constructing the interatomic interaction of a metal bond. This theoretical refinement makes it possible to calculate the values of ultrasound velocities in metals with high accuracy of the coinciding with the values of ultrasound velocities in metals, obtained experimentally on the basis of the molecular acoustics method, data about which are given in reference literature.

RESULTS AND DISCUSSION:

It is generally accepted to calculate the velocity of propagation of a longitudinal wave in a thin rod using the formula (Equation 1), where, υ_{cm} – velocity of propagation of a longitudinal wave in a thin rod, p – substance density, a E - Yung's modulus, determined on the basis of experimental data such as Equation (2). Here F – is the proportional component of the force; S – surface area over through which the force spreads; L – the length of the deformable rod; ΔL – modulus of change in the length of the rod as a result of elastic deformation.

Thus in the reference book (Anurev, 2001) the following data of the Yung's modulus for iron E = 200 GPa, and the density of iron p = 7830 kg/m^3. So, in accordance with the reference data according to Equation (1), we calculate the speed of sound in the rod (Equation 3). The resulting propagation velocity of the sound wave in the rod using the acoustic method is $\upsilon_{cm} = 5170$. It would seem that the error of the calculated and experimentally set speed is negligible (Equation 4).

However, Equation (1) is applicable under narrowly regulated conditions (does not take into account the “scale factor”) and does not reflect the process mechanics, which is determining the growth of the speed of ultrasonic waves in the process of elastic deformation of the rod, observed in practical research (Semukhin *et al.*, 2000). In other words, the proposed formula (model) does not fully reflect the mechanics of the process, which is determining the properties of the material and is not related to the structure of the crystal lattice of one or another metal.

According to O. Bravais's classification, iron has a body-centered cubic crystal lattice (Figure 1). The base of which is an elementary cubic cell, in which the positively charged metal ions are located at the vertices of the cube, and one more atom is in the center of its volume, that is, at the intersection of its diagonals (Prokhorov, 1998).

Considering the mechanism of sound velocity propagation in a metal, we will proceed from the fact that: "The vibrations of crystal lattice are one of the main types of internal motion of a solid, when the constituent of his structural particles (atoms, ions, molecules) oscillate around an equilibrium position - the nodes of crystal lattice (Prokhorov, 1998).

And since "... the interaction between atoms is final by quantity, then in the crystal there is a certain maximum frequency of oscillations $\omega_{\max}$ (usually $\omega_{\max} \approx 10^{13}$ Hz)" (Anurev, 2001). As a result, let's suppose that in the elementary cell of iron all atoms oscillate with the same frequency $\omega_{\max}$.

In work (Frenkel, 1972), Frenkel shows that "... in the case of sound waves, the wavelength is limited to the minimum value, which equals (approximately) to twice the distance between the atoms, which is associated with the discrete structure of the body ..." and is defined as Equation (5), whence the speed of sound propagation in the unit cell is defined as Equation (6).

So, as according to Equation (6), the speed passage of the wave depends on the wavelength and frequency, and appears possible to estimate the parameter α_{Fe} – the length of the edge of the unit cell of iron based on the experimental values of λ and υ.

In order to clarify the building of the crystal lattice, we use the determination of the size of the edge α_{Fe} on the basis of the parameters of the BCC lattice of the iron elementary cell, which were established by the method of X-ray structural analysis (Mitkevich, 1932). In order to clarify the building of the crystal lattice, we use the determination of the size of the edge on the basis of the parameters of the BCC lattice of the iron elementary cell, which were established by the method of X-ray structural analysis (Mitkevich, 1932). Figure 2 shows a schematic representation of an elemental volume-centered cubic cell of iron ABCDD`C`B`A` with a central atom located at the intersection of spatial diagonals. at the point O.

As can be seen from Figure 2, there are 2 atoms on the lateral verge of the edge AB, and the total length AB and the radius of the atom R_{atom} are determined by X-ray structural analysis and constitute, respectively, AB = $\alpha_{Fe} = 2.866 \cdot 10^{-10} m$ and $R_{atom} = 1.26 \cdot 10^{-10} m$. Calculate the distance between the electron shells of atoms, m (Equation 7), which will make Equation (8).

So, there is some distance Δ between the boundaries of the electron shells of atoms, through which the interaction takes place.

At the same time, the length of the spatial diagonal AC`, determined on the basis of the Pythagorean theorem, is equal to Equation (9) and after the expression in the sizes of the edge AB = α_{Fe} will get Equation (10) and, having made the further transformations, in the final form, the size of the diagonal of the lattice is defined as Equation (11) Next, substituting the value of the size of the atom $\alpha_{Fe} = 2.866 \cdot 10^{-10}$ = m, determine the size of the spatial diagonal of the crystal lattice (Equation 12).

However, according to the crystal lattice model (Figure 2), on this spatial diagonal should be located $4R_{atom}$, that is, the length of which should be equal to Equation (13).

As seen, the spatial diagonal of the AC `, calculated according to Equation (11), is smaller, then $4R_{atom}$. In this case, the atoms in this model must be overlapped by the electron shells or be in a deformed state. In fact, such a model leads to the fact that two different types of interaction between atoms should be observed in the one unit cell of iron:

• through the deformation of the electron shells of atoms (deformed by the central atom)

• the interaction of the electron shells of atoms, located at the top of the cube, occurs at a distance Δ, whose mechanism is unknown (Cohen, 1986).

In order to show that there is one common type of interatomic interactions in the unit cell of iron, and to eliminate the contradictions given above, let's clarify the presentation of "metallic bond" in the context of the notion about this type of bond by academician Ya.I. Frenkel. In his book, Ya.I. Frenkel (Frenkel, 1972) considers the interaction between two atoms depending on a certain distance r0, which are forming the total volume V0 of this interaction, in accordance with the scheme, showed in Figure 3.

Wherein, let us draw attention to the fact that, explaining the formation of the total volume of these two atoms, Frenkel points out: "These electrons, moving between atoms, provide a bond between them" (Frenkel, 1972). That is to say, that in fact, this is not about transmitting interaction through emptiness, but about some kind of mechanism for the movement of electrons in a common external orbit formed from the electrons of two neighboring atoms. The force of *attraction* of this diatomic system of Ya.I. Frenkel determines on the bases of the interaction of electric charges as Equation (14), where, e, kg $^{1/2}$ m$^{3/2}$ c^{-1} – is the electron charge; m, kg – is the electron mass; u, m / s – electron velocity; r, m – is the radius of the orbit of an electron in the Frenkel model.

Proton in view of its relatively large mass is considered immobile. Also Ya.I. Frenkel (Frenkel, 1972) clarifies: "Naturally, with an increase in the number of electrons (with a simultaneous increase in the charge of a positive ion), the force of gravity of electrons increases and the radius of the orbit decreases. As a result, the solidity of the bond increases." But he does not conduct a detailed consideration of the mechanics of the formation of a "collectivized" connection in his model. In this work, it is proposed to clarify the mechanism of formation of a diatomic model, based on the idea of the combining magnetic lines of force, given by Professor Mitkevich in the work (Mitkevich, 1932). For this, let's imagine the formation and hardening of a collectivized bond on account of the supposed transformation of electrons` orbits, similarly to the lines of force, as shown in Figure 4.

So, from Figure 4a it can be seen that at some distance r1 between the centers of two atoms there are no interaction forces. But when they approach at a distance r2 ‹r1, the valence atoms located on the outer orbit join (Figure 4b), and the electrons collectivize, forming some distance Δ, characteristic by that some internal orbits are at some distance Δ (Figure 4b) and do not interact between themselves. However, with a further decrease in the distance between the centers of the atoms r3 ‹r2‹ r1 (Figure 4c), repulsive forces of the same name charges in internal orbits appear, under the action of which the forces of attraction between atoms decrease.

Unification the outer, as well as the following after it, an electron orbit (Figure 4c), leads not only to a change in the force of attraction between the atoms due to an increase in the number of electrons participating in the formation of a bond, but also to the occurrence of anisotropy of properties into the direction of interatomic bond due to increase the amount of the constricting magnetic force lines. Wherein, in the proposed model, the parameters are r3. r2. r1 is greater than 2Ratom, and the presence of Δ satisfies both the conditions for the propagation of the speed of sound and the appearance of the forces of attraction and repulsion.

Thus, taking into account the introduced representation of the formation of an interatomic bond by means of constricting magnetic lines of

force, the nature and mechanism of the metallic bond in the unit cell can be explained. On the edge of the cell, it corresponds to the scheme of figure 4b, and in volume, the interplanar communication corresponds to the scheme of figure 4c, in connection with which it is necessary to accept that the spatial diagonal of the AC `should be slightly larger than 4Ratom (Equation 15). Therefore, comparing the spatial diagonal AC `with the size of the length of the edge of the unit cell α_{Fe} (11) will get that for the implementation of the condition (15), the new length of the edge of the unit cell must be greater than the spatial diagonal (Equation 16), where the value α_{Fe} must be Equation (17) or Equation (18).

Using the longitudinal sound velocity υ_{lt} = 5940 m / s, established empirically with the help of the acoustic method and the new parameter of the length of the edge of an elementary cell of iron equal to $\alpha_{Fe} = 3 \cdot 10^{-10}$ m, accepted with a certain excess of 2.5%, we calculate the frequency ω Fe of oscillations of iron atoms (Equation 19). Which, after substitution of numerical values, will be Equation (20).

Taking into account the existing definition (Prokhorov, 1998), "In those crystals, where each node is the center of symmetry, all normal waves are flat polarized: atoms in any normal oscillation make reciprocating - translational movements around their equilibrium positions", let's imagine the structure of the crystal through the interrelation of two elemental cells (Figure 5), which reflect both the structure and properties of iron.

Due to the homogeneity of the structure of the bulk-centered cell, this construction can be carried out at any vertex of the unit cell cube, which allows us to conclude that all waves in the elementary cell will be flat polarized and the atoms will perform normal oscillations around the equilibrium position in one plane (Regel *et al.*, 1974). Thus, to transfer an elastic oscillation under the action of an external pulse J_γ (Figure 2) from atom A to atom A`, when a transverse wave occurs, it is necessary to use two interatomic bonds: AO and OA ` (Figure 2), which will lead to increase τ the transmission time of the pulse (Equation 21).

Because of the fact that the distance of the interatomic bond between the central atom and the atoms located at the vertices of the cube are the same, then and the time of passage of ultrasound will be the same, and therefore we have the right to write the following expression (Equation 22). In this case, Equitation (21) will take the following value (Equation 23).

Accordingly, the velocity of the transverse wave υ_{tv} will be calculated as Equation (24), which after the substitution of numerical values – Equation (25) with an error of 0.9% can be taken equal to Equation (26).

Wherein, the transverse velocity obtained by an experimental way - by the method of molecular acoustics, is in the range of $\upsilon_{tv} = 3100 \pm 100$ m/s. Thus, the transverse velocity υ_{tv}, calculated through new parameters of the unit cell of the iron crystal lattice, almost coincides with the transverse velocity υ_{tv} obtained by the molecular acoustics method. As can be seen, the applicability of the calculation method through the refined lattice parameters of the iron elementary cell, which takes into account the structure of the crystal lattice, confirms the assumption about a single frequency $\omega_{\max}$ = Jdem oscillations of all atoms in the elementary cell of an iron. Whereas the existing model of the unit cell, as was shown above, reveals different manifestations of the oscillation frequency of the atoms in the same volume of the unit cell. In addition, the proposed model admits that the oscillation frequency of atoms under different loading conditions and temperature will be different, but the same for the entire cell volume of the material, therefore, that's why in accordance with the Van der Waals principle, it can be extended to the entire volume of the test material (Umansky *et al.*, 1955).

In order to show the constancy of the frequency of oscillation of atoms in the volume of the metal, we calculate the transmission rate of interaction between atoms from point A to point O (Figure 5) – Equation (27), from where Equation (28). This speed υ_{AO}, calculated at the same frequency as the longitudinal and transverse speeds, coincides with the speed of sound propagation in the rod $\upsilon_{cm} = 5170 м/с$, determined by the method of molecular acoustics. The difference is – Equation (29).

As can be seen, the refinement of the parameters of the crystal lattice made it possible to increase the accuracy of calculating the speed of sound in the rod, and also the direction of propagation of the speed of sound in the rod through the spatial diagonal was clarified. The

mechanics of this process can be explained in order, that the sound, when it falls on the surface of the rod, undergoes reflection, which leads to a kink of the vector of oscillations in the plane to the vector of oscillations in space, namely - along with the diagonal of the unit cell (Formalev *et al.*, 2016).

In accordance with the fact that, based on the refinements made, it was possible to determine all the velocities, by connecting the interatomic interaction distances with the speeds of sound propagation, we can write the general equation for calculating any velocity for a unit cell as Equation (30), where ℓ – is the length of the interatomic bond, expressed in terms of the edge parameter of the unit cell; ω – the frequency of oscillation of atoms in the unit cell; n – the number of interatomic interactions used to transmit sound in different planes of the unit cell. Moreover, Equation (30) is also true for the face-centered cubic elementary lattice ABCDD`C`B`A` (Figure 6).

To prove the validity of the proposed principle, by analogy with iron, we will calculate the theoretical rates for copper. Considering that the specified size of the face άCu depends on the fulfillment of condition (15), which is responsible for a single process of interatomic interaction, AB `> 4 • RCu, with RCu = 1,28 ·10^{-10}m, which was obtained through the X-ray-structured analysis, the size of the face of the face-centered cubic cell of copper should be larger (Equation 31). Then, with some assumption, we take that the new size of the copper face equal to Equation (32).

The total oscillation frequency of atoms in the cell of the copper ωCu will be found according to Equation (6), taking into account the value of the longitudinal velocity υ lt = 4700 m / s, which was set by the method of molecular acoustics (Equation 33), from where, after the substitution of numerical values, we will get Equation (34).

Given that there is the possibility of building a new one, second, unit cell EFKLL`K`F`E` in any vertex of the cube of the first unit cell, with the maintaining the size of the edge (Figure 6), the atoms in the face-centered cubic cell of copper will oscillate in one plane. In consequence of this, to transfer a transverse wave from atom A to atom A`, it is necessary to use two interatomic bonds AO and OA `. That is, substituting in Equation (27) the values n = 2; $L_{AA`}$ = 3.65 · 10^{-10}m and ω_{cu} = 1.28 • 10^{13} Hz, we will get Equation (35). Wherein, the transverse velocity in copper, established by the method of molecular acoustics, is equal to υtv = 2260 m/s. (The error was 3.9%)

The speed of sound in a copper rod υ AO, calculated in accordance with Equation (30), will be expressed as Equation (36), and when substituting the values of the length of the interatomic bond L AO and frequency will be Equation (37). At the same time, the speed of ultrasound in the rod, established in an experimental way, υAO = 3700 m / s (the error is 10%).

It is possible that this error is a consequence of the inaccuracy of determining the size of an atom and the length of the interatomic bond in the elementary cells of materials by the method of x-ray structural analysis. So when comparing the parameters of the unit cell of iron, obtained by X-ray-structural analysis (Chuprunov *et al.*, 2007), with the parameters of the unit cell of iron, obtained by calculation, the error is determined as Equation (38), where, ΔR_{Fe} – error between calculated radius and radius, based on the experimental values, R_{Fe} – radius of an atom of iron, based on the experimental values, R_{Fe}^{pac} – calculated radius of an atom of iron.

And will be Equation (39) or Equations (40, 41), where , $\Delta\alpha_{Fe}$ – error between calculated length of the edge of the unit cell of iron and length of the edge of the unit cell of iron, based on the experimental values, α_{Fe} – length of the edge of the unit cell of iron, based on the experimental values, α_{Fe}^{pac} – calculated length of the edge of the unit cell of iron.

In general, the error of X-ray structural analysis can be attributed to the fact that the oscillation frequency of X-ray waves is in the range $\upsilon_{x-ray} = 10^{16} - 10^{20}$ Hz (Berner and Kronmüller, 1968), whereby, the time of the fall of a wave on the surface of an atom will be $t = 10^{-16} - 10^{-20}$ s. During this period of time, the center of the atom, located at the point O (Figure 7), will shift relative to the equilibrium position by some amount $\pm\Delta x$. Then when accounting the longitudinal velocity $\vartheta_{\parallel} = 5940$ m/s and the time of the falling $t_1 = 10^{-16}$ s the displacement of the atom will be equal to $\Delta x_1 = \vartheta_{\parallel} \cdot t_1 = 6 \cdot 10^{-13} m$. What makes up half of the radius R_{Fe} or when accounting $t_2 = 10^{-20}$ s, will get $\Delta x_2 = \vartheta_{\parallel} \cdot t_2 = 6 \cdot 10^{-17} m$. And since the atom is in the mode of constant oscillation relative

to its center of an equilibrium (Figure 7), then at different times of the fall t_j the x-ray wave atom will shift at different distances relative to the center of oscillation, which will cause a change in the area of reflection from the Fe atom. In consequence of which, an error appears in determining the radius of the iron atom and the interatomic interaction parameter, which determines the edge length of the elementary iron cell.

CONCLUSIONS:

The analysis of the interatomic interaction mechanism of the diatomic model of Ya.I. Frenkel, on the basis of taking into account the process of interaction of the electron shells of atoms, made it possible to create a new model of the metallic bond, that refined the interatomic distances in the unit cell. In turn, this made it possible to associate the speed of the spread of sound with the structure of the crystal lattice and allowed us to carry out a theoretical calculation of the ultrasound velocities for different crystal lattices of metals.

The theoretically calculated values of the ultrasound velocities with a sufficiently high accuracy coincided with the experimental values of the ultrasound propagation velocities obtained by the molecular acoustics method. A theoretical explanation is given for the error in determining the size of atoms using method of X-ray diffraction analysis, which is associated with an increase in the reflecting surface due to the fluctuation of the atom, which makes it possible to verify the data of X-ray structuring analysis by the method of molecular acoustic.

The results obtained in this work open up the possibility of establishing a theoretical interrelation of the structure of crystal lattices of various metals with the physicomechanical properties of materials through the speed of spread of sound in this material, including under dynamic loads, what represents significant interest for non-destructive testing methods.

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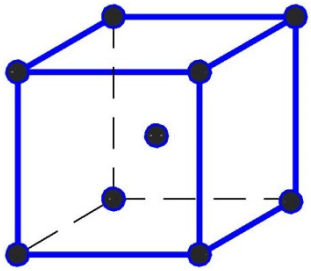

Figure 1. *Body-centered cubic crystal lattice (BCC) of Bravais*

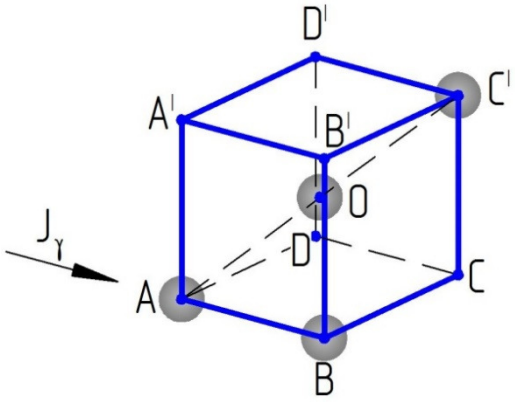

Figure 2. *The schematic construction of the iron elementary cell*

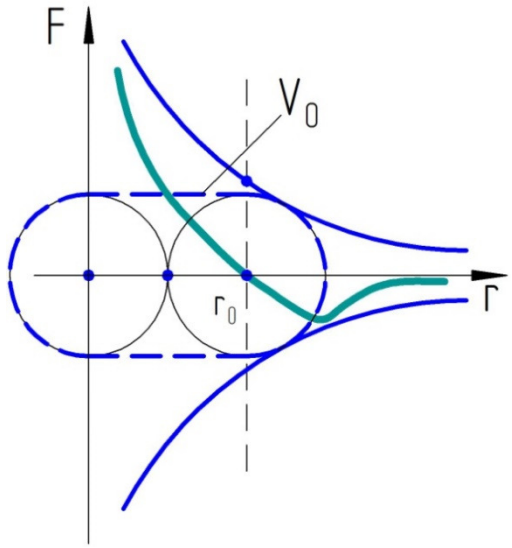

Figure 3. *The total volume V0, formed by two atoms in accordance with the model of Ya.I. Frenkel*

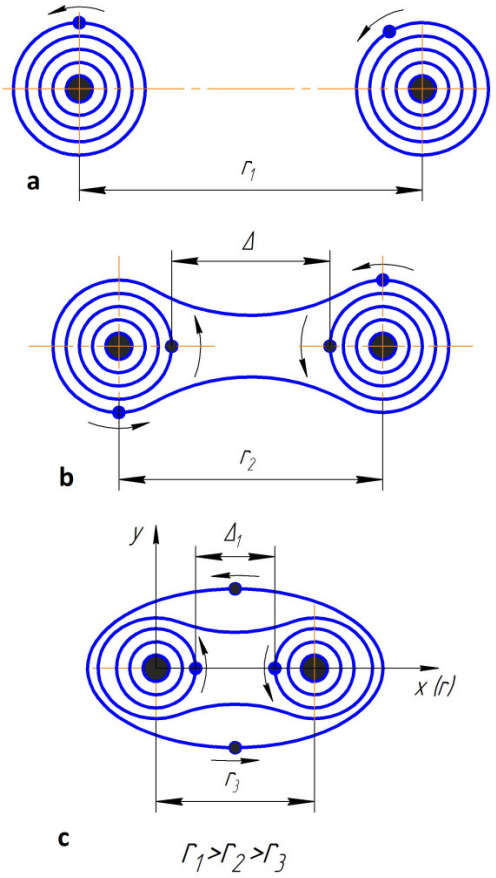

Figure 4. *Scheme of the formation of a metallic bond due to the transformation the orbits of electrons*

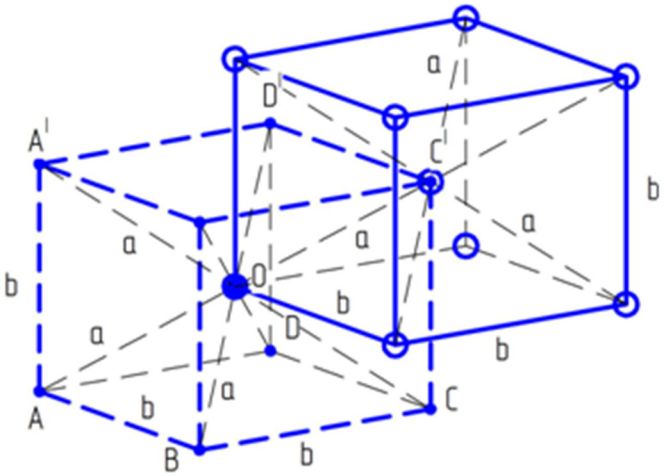

Figure 5. *The second (dashed) elementary cell is built at the top of the edge of the cube of the first one with the size of the edge length* $\alpha_{Fe} = 3 \cdot 10^{-10}$ *m*

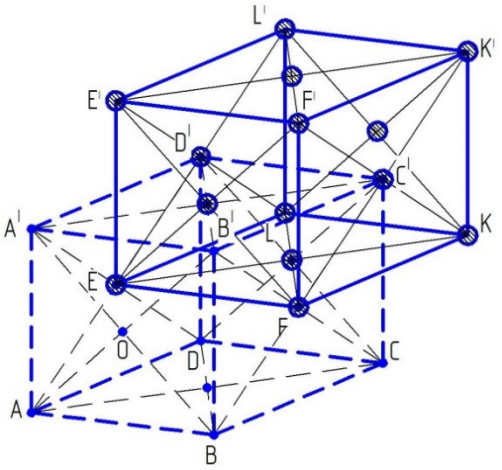

Figure 6. *An elementary face-centered cell EFRLL`K`F`E`, built at the top of the edge of the first face-centered cell ABCDD`C`B`A`*

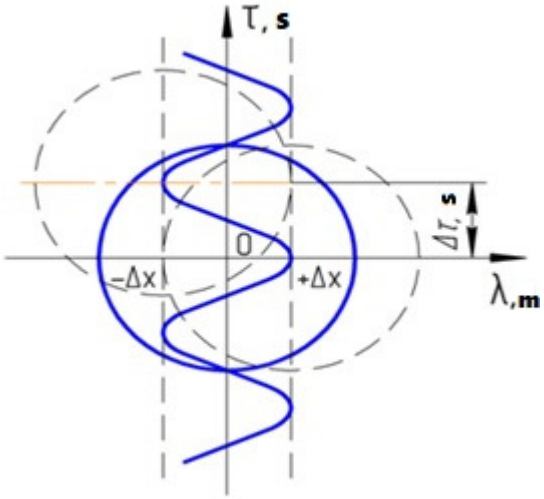

Figure 7. *The model of the "blurred" in time state of the atom in the unit cell*

$$\upsilon_{cm} = \sqrt{E/p}\ \text{, m/s} \quad (1)$$

$$E = [F/S]/[\Delta L/L]\ \text{, kg/m·s}^{2} \quad (2)$$

$$\upsilon_{cm} = \sqrt{200/7830} = 5060\ \text{, m/s} \quad (3)$$

$$\% = [(5170-5060)/5060]\cdot 100\% = 2{,}2\% \quad (4)$$

$$\lambda \approx 2 \cdot R_{atom}\text{, m.} \quad (5)$$

$$\upsilon \approx \lambda \cdot \omega_{\max}\text{, m/s} \quad (6)$$

$$\Delta = \alpha_{Fe} - 2 \cdot R_{atom}\text{, m,} \quad (7)$$

$$\Delta = 0{,}346 \cdot 10^{-10}\text{, m} \quad (8)$$

$$AC' = \sqrt{(AC)^2 + (CC')^2} \quad (9)$$

$$AC` = \sqrt{2\alpha_{Fe}^2 + \alpha_{Fe}^2} \quad (10)$$

$$AC' = \alpha_{Fe} \cdot \sqrt{3} \quad (11)$$

$$AC' = 2.866 \cdot 10^{-10} m \cdot 1.723 = 4.964 \cdot 10^{-10}\text{ m} \quad (12)$$

$$4R_{atom} = 4 \cdot 1.26 \cdot 10^{-10} = 5.04 \cdot 10^{-10} \quad (13)$$

$$Fgrav = e^2 / r^2 = m \cdot u^2 / r \quad (14)$$

$$AC` > 4R_{atom} \quad (15)$$

$$\alpha_{Fe} \cdot \sqrt{3} > 5.04 \cdot 10^{-10} m, \quad (16)$$

$$\alpha_{Fe} > 5.04 \cdot 10^{-10} m / 1{,}723 \quad (17)$$

$$\alpha_{Fe} > 2.925 \cdot 10^{-10} m \quad (18)$$

$$\omega_{\max} = \upsilon_{lt} / \alpha_{Fe} \quad (19)$$

$$\omega_{\max} = 5940 m/s / 3 \cdot 10^{-10}\ m = 1.98 \cdot 10^{13}, Hz \quad (20)$$

$$\sum t = t_{AO} + t_{OA`} \quad (21)$$

$$t_{AO} = t_{OA`} = 1/\omega_{\max} \quad (22)$$

$$\sum t = 2/\omega_{\max} = 2 / 1{,}98 \cdot 10^{13}\ Гц = 1{,}01 \cdot 10^{-13}\text{ (c)} \quad (23)$$

$$\upsilon_{tv} = AA` / \sum t \quad (24)$$

$$\upsilon_{tv} = 3 \cdot 10^{-10} m / 1.01 \cdot 10^{-13} = 2970{,}3 m/s \quad (25)$$

$$\upsilon_{tv} \approx 3000 m/s \quad (26)$$

$$\upsilon_{AO} = [(\alpha_{Fe} \cdot \sqrt{3}) / 2] \cdot \omega_{\max} \quad (27)$$

$$\upsilon_{AO} = 2.598 \cdot 10^{-10} m \cdot 1.98 \cdot 10^{13} Hz = 5144 m / s \quad (28)$$

$$\% = [(5170 - 5144) / 5144] \cdot 100\% = (26 / 5144) \cdot 100\% = 0.5\% \quad (29)$$

$$\upsilon = \ell \cdot \omega \cdot (1/n), \quad (30)$$

áCu > 3.62 ·10^{-10}m (31)

áCu = 3.65 ·10^{-10}m (32)

ω cu = υ lt / áCu (33)

ω cu = 1.28 ·10 ^{13} Hz (34)

υtv = 3.65 ·10^{-10}m ·1.28 ·10 ^{13} Hz· (1/2) = 2350 m/s (35)

υ AO = L AO· ω cu · (1/ n) (36)

υ AO =3.65 ·10^{-10}m ·(√2/2) ·1.28 ·10 ^{13}Hz· (1/1) = 3321 m/s (37)

$$\Delta R_{Fe} = [(R_{Fe} - R_{Fe}^{pac}) \cdot 100\%] / R_{Fe}^{pac}, (\%) \quad (38)$$

$$\Delta R_{Fe} = \frac{1.26 - 1.203}{1.203} \cdot 100\% = \frac{0.057}{1.203} \cdot 100\% = 0.047 \cdot 100\% = 4.7\% \quad (39)$$

$$\Delta \alpha_{Fe} = [(\alpha_{Fe}^{pac} - \alpha_{Fe}) \cdot 100\%] / \alpha_{Fe}, (\%) \quad (40)$$

$$\Delta \alpha_{Fe} = \frac{3 \cdot 10^{-10} - 2.866 \cdot 10^{-10}}{2.866 \cdot 10^{-10}} \cdot 100\% = \frac{0.114}{2.866} \cdot 100\% = 0.039 \cdot 100\% = 3.9\% \quad (41)$$