On the issue of determination of the mechanism of ultrasonic velocity change in the process of uniaxial deformation of the rod

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Abstract. The molecular acoustics method is one of the types of non-destructive testing of materials during the operation of machines and mechanisms. Assessment of the performance of this or that material for further operation is carried out on the basis of changes in the ultrasonic velocity passing through the volume of the material. In this case, this assessment is carried out on the basis of a comparison of experimental data with data on the change in the ultrasonic velocity (UV) in a rod made of the same material subjected to uniaxial deformation. Thus, this method correlates the value of the ultrasonic velocity in the material, after a certain operating time as part of a machine or mechanism, with one or another area of deformation of the rod. They try to explain the changes in the ultrasonic velocity on the basis of the displacement of defects or the rotation of mesoscopic volumes in the material. However, the authors describing in their works the process, use expressions "most likely", "probably", which indicates that their explanations are an assumption, and not a strictly established mechanism for changing the ultrasonic velocity. This work shows that in the process of deformation, together with a change of the ultrasonic velocity, both the natural frequency of atomic vibration and the volume of the primitive cell change. The author proposes to estimate the change in the ultrasonic velocity during deformation on the basis of changes in the geometric parameters of the primitive cell in which ultrasound is transmitted along the edges of the primitive cells through the interaction of electron shells of atoms.

Until now, iron (Fe) and alloys based on it remain the most used materials in industry and construction. The performance control of parts made of Fe and its alloys is carried out using non-destructive testing methods. One of these methods is molecular acoustics. "The main task of molecular acoustics is to study the structure and physical properties of gases, liquids and solids by acoustic methods" [1]. Therefore, on the basis of molecular acoustics, researchers are testing mathematical models in which they try to establish the relationship between the acoustic properties of a material, depending on its crystalline structure, and the changes occurring with it during deformation. To date, a large amount of experimental data has been accumulated on the change in the ultrasonic velocity in various materials during deformation. The main source for assessing the ongoing changes in the volume of the material is the analysis of experimental data on the change in the ultrasonic velocity obtained in the process of uniaxial tension of a rod made of the material under study. In the course of the experiments, the correspondence between the values of the ultrasonic wave velocity for different regions
of deformation is established. Figure 1 shows an experimental graph of the change of UV for low-carbon steel 09G2S deformed at the lower yield point obtained in [2].

Figure 2 and figure 3 show the experimental graphs of the UV changes for high-alloy steel 40X13 under active loading (strain rate $6.67 \times 10^{-5} \text{s}^{-1}$) of the samples in the state of delivery (figure 2) and after thermal annealing (high tempering $T^\text{C} = 600$) (figure 3) obtained in work [3].

The difference between the graph of low-carbon steel and the graphs for high-alloy steel is the presence of a small plastic deformation area and a hardening area. This is due to the conditions of deformation, or rather to the rate of deformation.

Figure 1. Experimental graph of the UV change during deformation of 09G2S steel at the lowest yield point.

Figure 2. Experimental graph of ultrasonic speed in 40X13 steel under active loading as delivered.

Figure 3. Experimental graph of ultrasonic speed in 40X13 steel under active loading after heat treatment.

Figure 4. Stresses for steel depending on the deformation rate.
"When a body is loaded above the elastic limit, the magnitude of plastic deformation is determined by the loading rate: the higher the loading rate, the shorter the time of plastic deformation and the greater the stress at which the transition from elastic to plastic deformation occurs" [4]. By changing the loading conditions of low-carbon steel, increasing the strain rate, it is possible to obtain identical stress profiles similar to high-alloy steel. This is confirmed by the theoretical studies of RI Nadeeva [5] (see figure 4) and the experiments of Meijong [6].

A characteristic feature of the graphs shown in figure 1-3 is the behavior of the ultrasonic velocity in the area of plastic deformation, which, according to the authors of [3], is characterized by the fact that "... at the parabolic stage, the velocity decreases in proportion to the total deformation." The authors of [3] offer an explanation of this dependence on the basis of dislocations: "The change in the ultrasonic velocity during deformation is determined by the behavior of mobile dislocations directly involved in the sliding process." A similar explanation is given by the authors of [2]: "... the reason for the decrease in the ultrasonic velocity, apparently, is the accumulation of defects such as dislocations and their ensembles as the total deformation increases." However, the authors of [2, 3] do not show the model of ultrasound transmission in the material, and also do not pay attention to the experimentally established fact that in the course of uniaxial tension of the rod, the natural vibration frequency of atoms changes both in the region of elastic deformation and in areas of plastic deformation. The authors of [7] clearly indicate: "The resonant frequency rises in the elastic and falls in the plastic area". If we take into account the model of Academician Ya.I. Frenkel [8] about the transmission of ultrasound by deformation of the electron shells of atoms, then an increase in the natural frequency $v_{at}$ of atomic vibrations in the elastic region of deformation will lead to an increase in the propagation velocity of ultrasound in the material. Decrease vat of the natural frequency of atomic vibration, in the plastic region, leads to a decrease in the propagation velocity of ultrasound in the material. That is, on the basis of the model of ultrasound transmission through the deformation of atomic shells, it is possible to explain the process of changing the UV during deformation, for this it is necessary to establish the reasons for the change in the natural frequency of atomic vibration.

In this regard, it is proposed to carry out a theoretical analysis of the change in the natural frequency of vibration of atoms $v_{at}$ and the UV of the wave $v$ under uniaxial tension on the basis of a set of known models - the model of the transmission of ultrasonic velocity by deformation of atomic shells, the model of the structure of primitive cells of the theory of O. Brave [9] and the model stress state as "... forced displacement of an atom from a position of stable equilibrium" [10]. It is proposed to focus on the analysis of changes in the parameters of the primitive cell of the crystal lattice in the process of deformation, since "... the process of deformation and destruction of solids cannot be understood without a specific analysis of the real structure of the body and its changes during loading" [11].

Let us carry out a theoretical analysis of the process of changing the UV during uniaxial deformation of a low-alloy steel rod. To do this, we represent the rod as a set of sequentially located one after another "backbones" of unit cells of the Body-Centered Cubic (BCC) crystal lattice, see figure 5.

![Figure 5. A rod as a sequence of N backbones of elementary cells located one after another with cell parameter $a$.](image)

In this case, the length of rod $L_0$ can be represented by the following expression

$$L_0 = N \times a$$  (1)
where \( a \) is the length (parameter) of the "backbone" of the unit cell of the BCC crystal lattice of iron. 

The area of elastic deformation of the rod, due to small relative deformations reaching 1-2%, can be represented as a sequential shift of atoms, in atomic planes from which a primitive cell is built [12], in the direction of the applied external force \( F_{\text{ext}} \) see figure 6

![Figure 6](image)

**Figure 6.** Deformation of the rod in the region of elastic deformation as a shift of atoms in atomic planes.

Then the new length of the rod, in the region of elastic deformation, will be expressed as

\[
L_{\text{elast}} = L_0 + \Delta L_{\text{elast}} = (a + \Delta x) \cdot N
\]  

(2)

and the relative elongation \( \Delta L_{\text{elast}} \) can be expressed from equation (2) by the following equality:

\[
\Delta L_{\text{elast}} = \Delta x \cdot N
\]  

(3)

To determine the change in the volumes of primitive cells in the area of elastic deformation, we will use the thermal research method. Let us assume that the process of stretching a rod in the region of elastic deformation occurs in such a short time interval \( \tau \) (c), that, in fact, this process can be attributed to an adiabatic process. Then, based on the adiabatic equation:

\[
T \cdot V^{(k-1)} = \text{Const}
\]  

(4)

where \( k > 0 \)

it can be found out that with adiabatic expansion of the body (increasing the volume of the rod \( V_\alpha \)), the body cools, and with adiabatic compression, the body heats up. Joule's researches [13] on uniaxial tension of the elastic rod made of iron found that the rod in the elastic deformation region cools a little. Nadai [14] directly points out that during adiabatic volumetric expansion of a solid body, heat is absorbed. Thus, on the basis of [13, 14], it can be argued that the volume of the rod \( V_\alpha \) increases. Taking into account the Van der Waals principle, an increase in the volume of the rod \( V_\alpha \) can be carried out only by increasing all volumes \( V_{\text{Cell}} \) "backbones" of unit cells of the BCC crystal lattice.

Let us assume that the increase in the volume of the "backbone" of the unit cell \( V_{\text{Cell}} \), in the elastic region of deformation, is carried out only by increasing the parameter of the interatomic distance \( a_{\text{BCC}} \) for some distance \( \Delta x \) in atomic planes along the vector of the applied external force \( F_{\text{ext}} \) while maintaining the geometric dimensions along the Y axis, as well as in the perpendicular plane (along the Z-axis). Figure 7 shows the deformation scheme of the "backbone" of a unit cell in the XY plane.
An increase in the length of the interatomic interaction (edge of the cell base) in the atomic plane leads not only to a change in the geometry and volume of the primitive cell $V_{Cell}$, but also to a change in the density of iron.

Currently, reference books indicate the values of the material density as the ratio of the mass of the $Mat_m$ to the volume of the primitive cell $V_{Cell}$. So the theoretical value of the density of iron is calculated based on the volume of the primitive cell of the BBC crystal lattice $V_{BBC}$

$$p_{ BBC} = \frac{M_{at}}{V_{BBC}} = \frac{9,3 \times 10^{-26} \text{Kg}}{11,69 \times 10^{-30} \text{m}^3} \approx 7955 \text{Kg/m}^3$$  (5)

The theoretical value of density, 7955 kg/m³, differs from the experimental value of density $\rho_{exper} = 7870$ kg/m³ by only 1%. However, the density of the iron atom

$$p_{at} = \frac{M_{at}}{V_{at}} = \frac{M_{at}}{\frac{4}{3} \pi R_{at}^3} = \frac{9,3 \times 10^{-26} \text{Kg}}{8,375 \times 10^{-30} \text{m}^3} \approx 11100 \text{Kg/m}^3$$  (6)

Thus, the true density of the physical element - Fe differs from the density of the crystal lattice of iron. However, if we take into account that the atom oscillates around the equilibrium position (crystal lattice node) with equal frequencies $\nu_x$ and $\nu_y$ along the X and Y axes, see figure 8, then for a certain interval (oscillation period) $T_0$, see figure 9, “the swept-out “volume $V_{swept}$, is formed see figure. 10. It is larger than the volume of the atom and only on the basis of the given movement of the atom, it is possible to refer the mass of the atom to the larger, swept-out volume.

$$p_{swept} = \frac{M_{at}}{V_{swept}} = \frac{M_{at}}{4 \pi R_{at}^3 \Delta x \Delta y}$$
Figure 10. Formation of a "swept-out" volume by $V_{\text{ zam}}$ atom, in the space of the crystal lattice, in one revolution of the center of mass of the O$_i$ atom near the crystal lattice node O.

However, then it is necessary to call the density of the given "swept-out" volume $V_{\text{ zam}}$ for the period $T_0$, the "time-distributed" density $\rho_t$.

To determine the changes occurring with the "distributed" density $\rho_t$ in the process of elastic deformation, we use the fundamental law of conservation of mass

$$m_{\text{ at}} = \text{Const}$$

where the mass of an atom remains unchanged in any primitive cell - deformed, not deformed during a polymorphic transition for any time interval $t_i$ at any frequency of atomic vibration $v_{\text{ at}}$ in any volume of a primitive cell $V_i$.

Based on the foregoing, about the conservation of the mass of an atom in any state of the material, we transform equation (7) as

$$\frac{m_{\text{ at}}}{V_i \ast \nu_i} = \frac{m_{\text{ at}}}{V_i} \ast \nu_i = \rho_t \ast \nu_i = \text{Const}$$

where $V_i$ is the volume of the cell
$\nu_i$ is the natural frequency of vibration of the atom
$T_i$ is the period of vibration of the atom
$\rho_t$ is "distributed in time" volume density

Suppose that equation (8) reflects the change in the "distributed" density of the material with a change in the primitive volume of the cell, as well as the change in the natural frequency of vibrations of the atom in the process of deformation. Let us write down the condition for the coherence of the initial parameters of the material with the parameters of the material in the region of the elastic deformation

$$\frac{m_{\text{ at}}}{V_0} \ast \nu_0 = \frac{m_{\text{ at}}}{V_i} \ast \nu_i = \text{Const}$$

where $V_0$ is the volume of the cell in the unloaded state
$\nu_0$ is the natural frequency of vibration of the atom
$V_i$ - volume of the cell in the area of elastic deformation
$\nu_i$ is the natural frequency of vibration of the atom in the region of elastic deformation.
We transform equation (9) by reducing the mass of the atom
\[
\frac{1}{V_0^*} \cdot V_{nat} = \frac{1}{V_i^*} \cdot V_{nat} = Const \left( \frac{1}{m^* c} \right)
\] (10)

Based on equation (10), it is possible to theoretically estimate the change in the natural frequency of vibration of the volume of the atom in the process of the elastic deformation. With an increase in the volume of a primitive cell, in the region of the elastic deformation, up to a new value \( V_i > V_0 \), the natural oscillation frequency of atom \( \nu_{iat} > \nu_{0at} \) should increase in order to preserve condition (10). Work [7] is the confirmation of the theoretical conclusions on the growth of the natural frequency of atomic vibration. The authors point out: "In our experiments, an increase in the frequency was always observed during the elastic deformation." Growth of the natural frequency of vibration of atoms \( \nu_{nat} \) can be explained by the change in the trajectory of the center of mass of the atom from a circle to an ellipse. It is known that when the amplitudes of two mutually perpendicular oscillations are equal, with equal frequencies, the point moves in a circle with a certain radius \( R_0 \) (see figure 8). With two mutually perpendicular oscillations of equal frequency but with different amplitudes and phase displacement, the movement of the point occurs along the ellipse with the semiaxes A and B, which lie in the directions corresponding to the oscillations, see figure 11.

![Figure 11. Changing the trajectory of the center of mass of an atom from a circle to an ellipse in the area of the elastic deformation.](image)

Thus, when the interatomic bond is deformed in the direction of the X axis under the action of an external force \( F_{ext} \), the trajectory of the center of the atom \( rO_1 \) changes to an ellipse. Taking into account that the period of oscillation of the center of atom \( T_0 \) should not change, then the speed of the center of the atom along the ellipse \( \nu_{el} \) increases in comparison with the same speed of the center of the atom circumferentially. This is due to the increase in the length of the perimeter of the ellipse in comparison with the perimeter of the circle. We find the speed of movement along the ellipse by formula

\[
\nu_{el} = \frac{2 \pi \sqrt{B^2 + A^2}}{T_0}
\] (11)

The length of semiaxis A is assumed to be equal to half of the length of the crystal lattice parameter in the elastic deformation region, taking into account the increase in the lattice parameter by 1% \( A = \frac{a \times 1.01}{2} = \frac{2 \times R_0 \times 1.01}{2} = 1.01 \times R_0 \) (12)

Knowing the turnover rate \( \nu_{el} \) of the center of atom point \( O_1 \), it is possible to determine, with some assumption, the new natural frequency of atom \( \nu_{nat} \) oscillation at point B relative to the node of the crystal lattice point O, assuming that point B is located on a circle with radius \( R_0 \)

\[
\nu_1 = \frac{\nu_{el}}{2 \pi \times R_0} = \frac{\sqrt{B^2 + A^2}}{\frac{R_0^2 + (1.01 \times R_0)^2}{2}} = \frac{R_0^2}{R_0 \times T_0} = \frac{1.005}{T_0}
\] (13)

Thus, in the region of the elastic deformation, the frequency of natural oscillations of the atom increases, which is explained by a change in the movement trajectory of the center of the atom relative to the node of the crystal lattice and the preservation of the turnover time (period \( T_0 \)) of the atom around the node of the crystal lattice.
An increase in the natural oscillation frequency of atom $v_i$ and an increase in the length of the crystal lattice parameter (the edge of the primitive cell) should lead to an increase in the velocity of the ultrasonic wave in the material. The value of the ultrasonic velocity in the elastic deformation region can be calculated by equation

$$\vartheta_{def} = l_i \cdot v_i \cdot \frac{1}{n} \ (\text{m/c})$$  \hspace{1cm} (14)$$

where $l_i$ is the length of the interatomic bond (the edge of the primitive cell) expressed in terms of the crystal lattice parameter - the length of the interatomic bond in the atomic plane.

$n$ - the number of interatomic bonds used for the transfer of ultrasonic energy in the plane and between adjacent parallel atomic planes forming the primitive and "backbone" of the elementary cell of the crystal lattice of the material.

Equation (14) was obtained in work [15] and allows only on the basis of the physical parameters inherent in the atom and the primitive cell of the crystal lattice to calculate the longitudinal, transverse and ultrasonic velocity in the rod. On the basis of this equation, in work [12], it was possible to refine the spatial design of primitive cells of BCC and Face-Centred Cubic (FCC) crystal lattices and introduce an additional requirement to the existing three requirements for choosing a primitive cell, on the passage of an ultrasonic wave along the interatomic bonds actually existing in space - the edges of the cell.

All changes - natural frequency, UV, volume of the primitive cell can be associated with the condition of continuity of the medium

$$\frac{n_{\text{ultr}} \cdot V_i}{V_i} = \text{Const} = \rho_i \cdot V_i \left( \frac{1}{M^* \cdot c} \right)$$  \hspace{1cm} (15)$$

where $\rho_i$ is the "time-distributed" density.

$V_i$ is the volume of the primitive cell at some point in time

$v_i$ is the vibration frequency of atoms in the volume of the primitive cell at the same time which remains until the destruction of the material. A joint analysis of equations (9), (10) and (15) can be carried out on the basis of the nomogram, see figure 12

In each of the quadrants of the Cartesian coordinate system, a constant hyperbolic function is presented. Point $O_1$ in the second quadrant corresponds to the initial conditions in the material before loading. An increase in the volume of the primitive cell (point $A_1$) under the action of external forces in the area of the elastic deformation corresponds in the first quadrant (point $A$) to an increase in the natural oscillation frequency of the atom, which corresponds to [7], and a decrease in the values of the "distributed" density.

**Figure 12.** Nomogram of changes in the distributed density, primitive volume, and natural vibration frequency of atoms under loading.
Then, taking into account the fact that in the region of the plastic deformation [7], the natural oscillation frequency of the atom decreases, one can identify point B in the first quadrant as a region of the plastic deformation. As a consequence, point B1 (display of point B) in the second quadrant indicates a decrease in the primitive volume of the cell in comparison with the initial parameter. A decrease in the primitive cell volume \( V_{\text{cell}} \) is possible with the all-round compression of the body or with the rearrangement of atoms in atomic planes under the uniaxial deformation, see figure 13.

![Figure 13. Rearrangement of atoms in the atomic plane into a region with low potential energy during deformation.](image)

The process of the rearrangement of atoms, in atomic planes, corresponds to the mechanism of occupying space with a minimum potential energy [10], i.e., the movement of atoms into the \( S_{\text{min}} \) region, see figure 13. This changes the parameter of the primitive cell. In accordance with work [15], the diagonal of the resulting crystal lattice must meet the requirement

\[
a \ast \sqrt{2} \geq 4 \ast R_{a1}
\]

which results in value \( a \geq 3.564 \times 10^{-10} \text{M} \). The closest actually existing value of the "backbone" parameter of the elementary crystal lattice of iron, satisfying condition (16), is the parameter of the FCC crystal lattice. Figure 14 shows the "backbones" of BCC and FCC cells consisting of primitive cells given from work [12].

![Figure 14. "Backbones" of unit cells of the crystal lattice formed from three parallel atomic planes \( \alpha, \beta \) and \( \gamma \).](image)

The existence of FCC crystal lattice, that is, the transformation of primitive cells from \( \alpha \text{Fe} \) to \( \gamma \text{Fe} \), is confirmed by [17, 18]. "At pressures above 105 kg/cm2, a polymorphic transition was found in iron by measuring the compressibility at the shock front." [18]. A theoretical analysis of the change in the natural frequency of atomic vibration \( \nu_{\text{at}} \) during the transformation of primitive cells from \( \alpha \text{Fe} \) to \( \gamma \text{Fe} \) was carried out in [16], in which the dependence of \( \nu_{\text{at}} \) on the coordination number \( K \) was established.

\[
\frac{V_{\text{BBC}}}{V_{\text{BCC}}} = \frac{V_{0_{\text{BBC}}}}{V_{0_{\text{BCC}}}} \frac{K_{\text{BBC}} \cdot V_{\text{BCC}}}{K_{\text{HBC}} \cdot V_{\text{HBC}}}
\]

where \( V_{0_{\text{BBC}}} \) is the volume of the primitive cell of the BCC crystal lattice

\( K_{\text{BBC}} - \) coordination number of the BCC cell
ν\textsubscript{BCC} is the oscillation frequency of atoms in a primitive BCC cell

\( V_0 \text{HBC} \) - the volume of the primitive cell of the FCC crystal lattice

\( K \text{HBC} \) - coordination number of the FCC cell

ν\textsubscript{HBC} is the oscillation frequency of atoms in a primitive FCC cell.

It was found from equation (17) that the oscillation frequency of the atom in a primitive cell of the FCC crystal lattice decreases in comparison with the natural oscillation frequency of atoms in a primitive cell of the BCC crystal lattice

\[
\nu_{\text{HBC}} \approx \frac{2}{3} \nu_{\text{BCC}}
\] (18)

Thus, in the process of the theoretical analysis, it was found that the reasons for the change in the natural vibration frequency of atom \( \nu \) are the change in the position of the atom in the space of the atomic plane both in the elastic region of deformation and in the plastic region of deformation. A change in the position of an atom in the atomic plane changes the spatial structure of the primitive cell, which leads not only to a change in the volume of the primitive cell, but also to a change in coordination number \( K \) characterizing the spatial configuration of the arrangement of atoms.

To clarify the characteristics (graph) of the change in the UV in the plastic region of deformation, let us consider, from a theoretical point of view, the process of polymorphic transformation of cells from \( \alpha \text{Fe} \) to \( \gamma \text{Fe} \) for a certain time interval \( \Delta \tau \) during uniaxial deformation of the rod in the plastic region. Let the rod, in the region of elastic deformation, consist of \( N \) successively deformed BCC cells and at time \( \tau_0 \) the first polymorphic transformation (plastic deformation begins) of the vertical plane occurs, see figure 15.

![Figure 15. Timepoint \( \tau_0 \).](image)

For a certain period of time \( \Delta \tau = \tau_1 - \tau_0 \), a rearrangement of \( P \) vertical planes will occur, see figure 16.

![Figure 16. Time moment \( \tau_1 \).](image)

Most likely, the rearrangement does not occur sequentially, as shown in figure 16, but on defects of the crystal lattice, where the potential energy is minimal; however, to simplify the theoretical analysis, we will consider the rearrangement of cells occurring one after another, sequentially.

The UV of the wave in the rod in the region of the elastic deformation can be presented as

\[
\mathcal{G}_{\text{el}}(\omega) = \frac{L_{\text{el}}}{\omega} = \frac{N \star \nu_{\text{BCC}}}{N \star \nu_{\text{BCC}}}
\] (19)

where \( L_{\text{el}} \) is the length of the bar in the area of the elastic deformation.
\( \tau_{\text{BBC}} \) is the time of passage of an ultrasonic wave of one length of the edge of the primitive cell in the region of the elastic deformation.

\( a_{\text{BBC}}^1 \) is the length of the edge of the primitive cell in the area of the elastic deformation.

The length of the rod at the polymorphic transition from \( \alpha \text{Fe} \) to \( \gamma \text{Fe} \) can be expressed by the following sum

\[
L_{\text{st}(\text{plast})} = (N - P) \cdot a_{\text{BBC}}^1 + P \cdot a_{\text{HBC}}
\]

where \( N \) is the initial number of cells of the FCC crystal lattices forming the length of the rod in the region of the elastic deformation.

\( P \) is the number of cells of fcc crystal lattices formed in the rod during polymorphic rearrangement in the region of the plastic deformation.

\( a_{\text{BBC}}^1 \) is the length of the edge of the BCC crystal lattice in the elastic deformation region.

\( N \) \( a_{\text{HBC}} \) is the length of the edge of the FCC crystal lattice.

Then the total time of passage of the ultrasound by the wave of the material through different structural units, different crystal lattices, can be expressed as

\[
\sum \tau^i = (N - P) \cdot \tau_{\text{BBC}}^i + P \cdot \tau_{\text{HBC}}
\]

\( \tau_{\text{BBC}} \) is transit time of 1 cell of the BCC crystal lattice.

\( \tau_{\text{HBC}} \) is the transit time of 1 FCC cell of the crystal lattice.

Accordingly, the UV of the wave in the rod in the region of plastic deformation will be expressed as

\[
\mathcal{g}_{\alpha(\text{plast})} = \frac{L_{\text{st}}}{\sum \tau^i} = \frac{(N - P) \cdot a_{\text{BBC}}^1 \cdot a_{\text{HBC}}^1 + P \cdot a_{\text{HBC}}}{(N - P) \cdot \tau_{\text{BBC}}^1 + P \cdot \tau_{\text{HBC}}}
\]

Let us estimate the change of the UV according to equation (22) at two extreme points \( P = 0 \) and \( P = N \).

\[
\mathcal{g}_{\alpha(P=0)} = \frac{(N - 0) \cdot a_{\text{BBC}}^1 + 0 \cdot a_{\text{HBC}}}{(N - 0) \cdot \tau_{\text{BBC}}^1 + 0 \cdot \tau_{\text{HBC}}} = \frac{a_{\text{BBC}}^1}{\tau_{\text{BBC}}^1} = \mathcal{g}_{\text{BBC}}^1
\]

\[
\mathcal{g}_{\alpha(P=N)} = \frac{0 \cdot a_{\text{BBC}}^1 + N \cdot a_{\text{HBC}}}{0 \cdot \tau_{\text{BBC}}^1 + N \cdot \tau_{\text{HBC}}} = \frac{a_{\text{HBC}}}{\tau_{\text{HBC}}} = \mathcal{g}_{\text{HBC}}
\]

The UV of the wave in the rod will correspond to the speed of sound in the deformed bcc crystal lattice \((\mathfrak{v}_{\text{Elast.def.BBC}})\). At \( P = N \), the ultrasonic velocity will be equal to the UV in the FCC crystal lattice.

\[
\mathcal{g}_{\alpha(P=N)} = \frac{0 \cdot a_{\text{BBC}}^1 + N \cdot a_{\text{HBC}}}{0 \cdot \tau_{\text{BBC}}^1 + N \cdot \tau_{\text{HBC}}} = \frac{a_{\text{HBC}}}{\tau_{\text{HBC}}} = \mathcal{g}_{\text{HBC}}
\]

Based on the two extreme points, taking into account the uniform gradual transition of primitive cells from \( \alpha \text{Fe} \) to \( \gamma \text{Fe} \), we construct a theoretical graph of the change of the ultrasound in the rod, see figure 17.

\[
\text{Figure 17. Theoretical change of the UV during polymorphic rearrangement of primitive cells from } \alpha \text{Fe to } \gamma \text{Fe.}
\]

Thus, the UV in the rod decreases in proportion to the number of changing crystal lattices of cells from BCC to FCC. Accordingly, knowing the mechanisms of speed change in the area of elastic and plastic deformation, it is possible to construct a theoretical graph of the change of the UV in the rod, see figure 18.
Figure 18. Theoretical graph of the change in the ultrasonic velocity in the rod during active loading.

The region of elastic deformation OA is an increase of the UV from value $\nu_0$ to the velocity value in the elastic region $\nu_{Elast.def.BBC}$. The area of plastic deformation AB is the drop of the UV. Point A1 corresponds to $P = 0$, and point B1 corresponds to some intermediate value $P = M$ of polymer transitions of crystal lattices from $\alpha$Fe to $\gamma$Fe. In the region of plastic deformation (parabolic stage of stress), the UV decreases in proportion to the relative elongation, i.e. proportional to the growth in the number of changing crystal lattices BCC-FCC ($P - M$) to a certain value of the UV $\nu_{plast} (f (M))$.

Thus, the theoretical graph of the change of the UV in the rod made of iron, with the uniaxial deformation, has the same profile with the graphs shown in figure 2 and figure 3. This can be explained by the fact that the substitution of iron atoms for chromium atoms in the crystal lattice of 40X13 steel does not change the type of the crystal lattice, since both materials have the same BCC crystal lattice, with practically the same value of the crystal lattice parameter $a_{Cr} = 2.855 \times 10^{-10} M \cdot a_{Fe} = 2.866 \times 10^{-10} M$.

The radius of the chromium atom $R_{Cr} = 1.3 * 10^{-10} m$ is approximately equal to the radius of the iron atom $R_{Fe} = 1.26 * 10^{-10} m$ (the difference is 3%). The valence of chromium and iron is the same. Also, the values of the ultrasonic velocity in the rod almost coincide $\nu_{Cr} = 5140 m / s$ and $\nu_{Fe} = 5170 m / s$. Therefore, the deformation of the crystal lattice in the elastic deformation region and the polymorphic transformation from $\alpha$Fe to $\gamma$Fe with chromium atoms in the plastic region should be identical, which is confirmed by the coincidence of the theoretical graph of the ultrasonic velocity change with the experimental ones.

A theoretical analysis of the change of the wave ultrasonic velocity, based on the model of ultrasound transmission by deformation of the shells of atoms, along the edges of primitive cells of the crystal lattice of iron and their changes, during uniaxial deformation of the rod, shows that all changes of the UV are associated with the change in the natural oscillation frequency of atom $\nu_{0}$, which changes during the deformation of the interatomic bond, which is associated with the change in the trajectory of the center of mass of the atom near the node of the crystal lattice. In turn, the change in the motion of the center of mass of the atom is associated with the condition for the formation of "distributed" density $\rho_{d}$ of the material, that is, the condition of continuity of the medium, which is expressed by the equation for the region of elastic deformation

$$\rho_{0} * \nu_{0} = \rho_{1} * \nu_{1} = Const = \frac{\rho_{L}}{\tau_{i}} \quad (25)$$

Equation (17), which reflects the process of changing the "distributed" density during the polymorphic transformation of primitive cells (plastic flow regions), can be transformed into a similar equation, if the following mathematical transformations are carried out

$$\frac{\rho_{BBC} * V_{0BBC}}{\rho_{HBC} * K_{BBC} * V_{BBC}} = \frac{\rho_{HBC} * V_{0HBC}}{\rho_{HBC} * K_{HBC} * V_{HBC}} \quad (26)$$

$$\frac{M_{at}}{\rho_{BBC} * K_{BBC} * V_{BBC}} = \frac{M_{at}}{\rho_{HBC} * K_{HBC} * V_{HBC}} \quad (27)$$
with a reduction in the mass of the atom in both parts of the equality, it is possible to obtain the final equality of the distributed densities for primitive cells of the BCC and FCC crystal lattices

\[
\rho_{\text{BBC}} \cdot V_{\text{BBC}} \cdot K_{\text{BBC}} = \rho_{\text{HBC}} \cdot V_{\text{HBC}} \cdot K_{\text{HBC}} = \text{Const}
\]  

Equation (28) differs from equation (25) only by taking into account the coordination number \(K\). The coordination number \(K\) indicates that the formation of the "distributed" density of the BCC primitive cell \(\rho_{\text{BBC}}\) and the FCC primitive cell \(\rho_{\text{HBC}}\) involves the near neighboring atoms. Figure 19 shows a diagram of the formation of a "distributed" density of a primitive cell of a material by neighboring atoms.

![Figure 19. Overlapping of the same volume by neighboring atoms during oscillation period \(T_0\).](image)

by overlapping the same volume of the primitive cell for one period of oscillation \(T_0\), but at different points in time of this period.

Equation (25), reflecting the change in the "distributed" density in the elastic deformation region, should be supplemented with the coordination number \(K_{\text{BBC}}\), which reflects the participation of neighboring atoms in the formation of the volume of the primitive cell of the BCC crystal lattice

\[
K_{\text{BBC}} \cdot \rho_0 \cdot V_0 = K_{\text{BBC}} \cdot \rho_1 \cdot V_1 = \text{Const}
\]  

Thus, all changes in the ultrasonic wave velocity during uniaxial deformation of the rod are explained on the basis of the continuity condition of the medium and are reflected in the nomogram in figure 12. Defects in the crystal lattice (such as vacancies) do not transfer the energy of the ultrasonic wave. However, vacancies are regions with low potential energy and it is easier for atoms to displace precisely to this region upon deformation under the action of the external force; therefore, the polymorphic transition is most likely to begin precisely on the voids (vacancies) of the crystal lattice. It should be noted that the theoretical graph of the change of the UV shown in figure 18 will depend on the deformation rate of the rod. In this case it coincides with the active loading of the steel (the deformation rate is \(6.67 \times 10^{-5}\) s\(^{-1}\)). The process of the material deformation as a displacement of atoms in atomic planes, depending on the loading rate, will be considered in a separate work.

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