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A method for theoretical calculation of Young's modulus and modulus shear for metals and their alloys under normal conditions based on a new model of sound wave transmission in metal

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Abstract. The paper presents theoretical calculations of the values of Young's modulus and shear modulus for single crystals of iron, chromium, and other metals and alloys based on a new model of sound transmission in metals. The theoretical values of Young's modulus and shear modulus obtained for undeformed metals under normal conditions are slightly less than the values of Young's modulus and shear modulus for these materials obtained experimentally, which is consistent with the condition of stress growth during elastic deformation.

1 Introduction

The process of elastic deformation of metals has been studied for over a hundred years. Analysis of changes in physical and mechanical properties, as well as changes in the crystal lattice of the material, is carried out based on various methods - X-ray structural analysis, thermal analysis, molecular analysis and others. Each research method has its own paradigm - a set of theoretical and methodological provisions, that is, its own specific mathematical model. Thus, several different mathematical models are used to study the same deformation process, which leads to the "splitting" of the general, inherent in nature, physical process into parts. Therefore, the main task of materials science at present is to find a common concept (physical model), the "foundation" of which would be the idea of the interatomic bond, and it is on the changes occurring in the interatomic bond that various data (change in temperature, change in the speed of sound, change in voltage) obtained on the basis of various assessment methods are explained. The criterion for evaluating such a physical model should be the principle of sufficient reason, which was formulated by Leibniz as follows: it is possible to assert the existence of an entity, phenomenon, connection, pattern, etc. only if there are grounds, that is, facts (experimental data) or logical conclusions from facts (experimental data) that confirm this judgment. Considering simple and complex explanations from the point of view of this principle, it is easy to see that if a simple explanation is complete and exhaustive, then there are simply no sufficient grounds for introducing additional components into the reasoning [1].

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2 Materials and methods

The work [2] proposed a physical model of interatomic interaction for metals. According to this model the force of attraction of atoms in monatomic planes and between them is carried out by “magnetic” loops (see Figure 1).

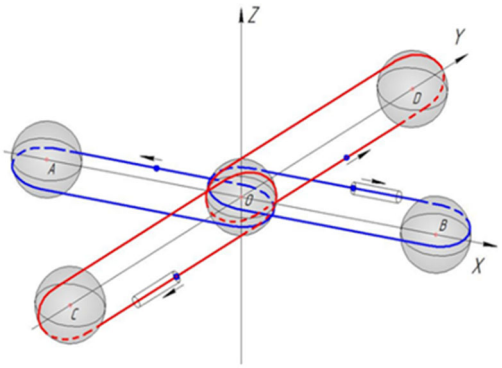

Fig. 1. Model of attraction of neighboring atoms by "magnetic" loops in monatomic planes.

The “magnetic” loop itself has a dedicated volume in the interatomic space, which is formed due to the attraction of rotating $n_e$electrons, which have circumferential $\upsilon_\omega$and longitudinal $\upsilon_p$velocities (see Figure 2).

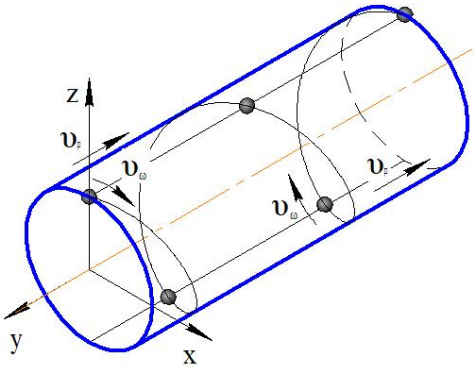

Fig. 2. Model of formation of the volume of the "magnetic" loop.

Based on this model, the work [2] managed to explain, from a theoretical point of view, the physical process of increasing the speed of sound propagation in metals [3] occurring in the region of elastic deformation with a decrease in the temperature of the sample [4,5], and also to explain the decrease in the speed of sound during heating (with an increase in the natural frequency of oscillation of the atom) and an increase in the speed of sound during cooling of the metal [6] (with a decrease in the natural frequency of oscillation of the atom) without deformation. This model also explains the physical process of the occurrence of a temperature gradient [5] in a sample during elastic loading of the sample with two equal and oppositely directed moments that create its uniform bending along the length (stretched fibers parallel to the axis of the rod will cool slightly, and compressed ones will heat up slightly compared to the initial unloaded state).

All these processes were explained by accepting that the energy of the interatomic bond (the energy of the "magnetic" loop) is a constant value$E_{m.l} = Const$, and the energy of the

sound wave E_λ in the metal propagates in the volume of the loop with the longitudinal velocity of the electron v_p. However, in this model the number of electrons n_e in the magnetic loop was not specified. If the number of electrons in the "magnetic" loop is specified, this will allow us to calculate the theoretical value of the attractive force f_e between the electrons and, accordingly, the internal voltage σ_e in the magnetic loop. To calculate the theoretical value of voltage in metals, the following theoretical equation was proposed in [7]:

$$\sigma = \frac{f_e}{S} = \frac{e^2}{a^4} \quad (1)$$

on the basis of which an approximate estimate of the internal "zero" stress in metals is obtained. The approximate estimate according to formula (1) is due to the fact that the parameter a, the parameter of the crystal lattice, is taken as the distance between electrons, and on the other hand, as the area $S_e = a^2$ on which the force of attraction of electrons is formed in accordance with another equation given by Frenkel in his work [7]:

$$f_e = \frac{e^2}{a^2} \quad (2)$$

Given the current understanding that "collectivized" electrons are randomly distributed within the volume of a primitive cell and throughout the entire crystal lattice, it is important to examine the rationale behind the distance a between electrons being set as in equation (2). Additionally, the basis for the area a^2 of interaction of electrons should be considered. Clarifying expressions (1) through a new model of interatomic interaction involving "magnetic" loops may provide valuable insights into these aspects.

$$\sigma_e = \frac{e^2}{b^2{}_e * S_e} \quad (3)$$

where b_e is the distance between electrons in a "magnetic" loop; S_e is the loop area; we will be able to obtain a value of internal stress σ_e equal to or slightly less than the value of Young's modulus determined by uniaxial deformation of the rod. Therefore, it is proposed to carry out a theoretical calculation of the values of Young's modulus E and shear modulus G according to equation (3) for single crystals of iron, chromium, other metals and their alloys with different structures of crystal lattices.

3 Results and discussion

To establish the number of electrons n_e in the loop, we assume that the external energy, which depends on the external temperature, is absorbed (emitted) into the metal crystal lattice by the "magnetic" loop in the form of electron energy quanta. Thus, it is necessary to establish the additional mass Δm_{at} introduced into the volume of the primitive cell of the substance's crystal lattice with an increase in external temperature from -273Cº to 20Cº. It is known [8] that the theoretical mass of an atom m_{at} can be determined based on the number of conventional units $N_{a.e.m}$ (atomic mass units) as follows:

$$m_{at} = N_{a.e.m} * m_{a.e.m} \quad (4)$$

where $m_{a.e.m} = 1{,}660539066 * 10^{-27} kg$.

Let us assume that equation (4) corresponds to the determination of the mass of an atom at a temperature of absolute zero T = -273º C. And we will determine the mass of an atom under normal conditions (20±0.1 º) based on reference data on the density of matter ρ, which is determined under the same normal conditions based on the equation (5):

$$m_{at} = \rho(20°C) * V_{cell}/n \quad (5)$$

Volume of the unit cell $V_{cell} = a^3$; n - the number of atoms per unit cell volume [9]; a - the length of the edge of the unit cell of the cube of the substance determined by X-ray structural analysis at 20±0.1 º . Having determined the masses of atoms of one element at different temperatures, it will be possible to find the difference in masses at different temperatures.

$$\Delta m_{at} = m_{at}(20^{\circ}C) - m_{at}(-273°C) \quad (6)$$

Let us first consider the data given in the reference book [15] for iron Fe. The lattice parameter of iron under n. c. is $a_{Fe} = 2{,}886 * 10^{-10}$m, the density of iron is $\rho_{Fe} = 7870$kg/m^3. The mass of an iron atom can be determined from these conditions as:

$$m_{at} = \rho * V_{яч} * \frac{1}{n} = 7870 \frac{кг}{м^3} * (\frac{1}{2}) * (2{,}866 * 10^{-10}м)^3 = 92{,}634 * 10^{-27} kg \quad (7)$$

The mass of an atom calculated from (4) is:

$$m_{at} = 55{,}845 a.e.m * 1{,}660539066 * 10^{-27} \frac{kg}{a.e.m} = 92{,}732804 * 10^{-27} kg \quad (8)$$

It can be seen that the value of the mass of an atom at absolute zero (8) is greater than the mass of an atom under n. c. (7). However, this cannot be like this. It is known [14] that: "The mass of a body is a measure of the energy content of this body; if the energy changes by the value L, then the mass changes accordingly by the value $L/9\times10^{20}$, and here the energy is measured in ergs, and the mass is in grams ...". Thus, when heated, the energy of the body increases, therefore the mass of the metal also increases. It is necessary to remember that the dimensions of the body change depending on the temperature - they increase when heated and decrease when cooled [14]. It is also necessary to understand that an oscillating atom in a crystal lattice node creates a large reflection area, which, during X-ray structural analysis, affects the established dimensions of both the radius of the atom and the edge size a_{Fe} of the iron crystal lattice. Thus, there is a need to clarify the parameter a_{Fe} of the crystal under n. c. In the work the principle of a single interatomic interaction in the elementary cell for all atoms forming any elementary (primitive) cell of the crystal lattice was introduced – the existence of a distance Δ between the shells of atoms. Thus, the spatial diagonal $l_{1\text{-}0\text{-}6}$ must be greater than 4 radii of an iron atom R_{at}^{Fe} (see Figure 3).

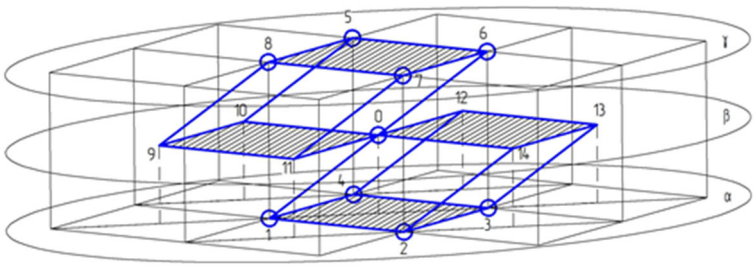

Fig. 3. The skeleton of the "elementary" 0-1-2-3-4-5-6-7-8 BCC cell of the crystal lattice, formed from three parallel atomic planes α, β and γ.

Let us write this equation as follows:

$$a_{Fe} * \sqrt{3} \succ 4 * R_{at}^{Fe} \quad (9)$$

from which a new value a_{Fe} of the crystal lattice parameter can be established. Let us assume that the radius of the iron atom $R_{at}^{Fe} = 1{,}26 * 10^{-10}m$, established by X-ray structural analysis, is sufficiently accurate - then the new parameter of the iron crystal lattice should exceed the value

$$a_{Fe}^{1} \succ 4 * 1{,}26 * 10^{-10}(m)/\sqrt{3} = 2{,}9099 * 10^{-10}(m) \quad (10)$$

Let us accept a new value $a_{Fe}^{1} = 2{,}915 * 10^{-10}(m)$, which will allow the existence of a gap $\Delta_1 = 0{,}395 * 10^{-10}(m)$ between atoms in atomic planes and a gap $\Delta_2 = 0{,}0044 * 10^{-10}(m)$ between atoms on the spatial diagonal AOD, in parallel monatomic planes, see Figure 4, from which the "skeleton" of the elementary cell is formed.

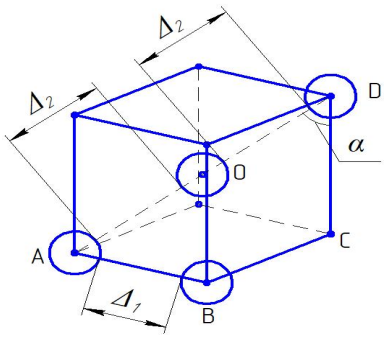

Fig. 4. The "skeleton" of the elementary cell of the iron crystal lattice.

Having specified the parameter of the iron crystal lattice a_{Fe}^{1}, we calculate the value $m_{at}^{Fe}(20°C)$:

$$m_{at}^{Fe}(20°C) = 7870\,\frac{kg}{m^3} * \frac{1}{2} * (2{,}915 * 10^{-10}(m))^3 = 97{,}467631 * 10^{-27}(kg) \quad (11)$$

The additional mass Δm_{at}^{Fe} will be:

$$\Delta m_{at}^{Fe} = 97{,}467631 * 10^{-27}(kg) - 92{,}73280414 * 10^{-27}(kg) = 4{,}734827 * 10^{-27}(kg) \quad (12)$$

Given the value of the electron mass, equal to $m_e = 9{,}109 * 10^{-31}(kg)$, we calculate the additional number of electrons $\sum n_e$ located in all "magnetic" force loops belonging to 1 atom:

$$\sum n_e = \frac{\Delta m_{at}^{Fe}}{m_e} = \frac{4{,}734827*10^{-27}(kg)}{9{,}109*10^{-31}(kg)} = 5197{,}9 \approx 5198(things) \quad (13)$$

It should be noted that this number of electrons $\sum n_e$ calculated in (13) will belong to each atom in the entire iron crystal lattice since the density of the substance is determined for the entire volume of the material. Having obtained the value of the number of additional electrons per 1 atom, it is necessary to distribute them in the "magnetic" loops (interatomic bonds), of which the iron atom, according to valence, has only 6. Let us consider Figure 3. The central atom No. 0 located in the β plane, which is the top of the primitive cell 1-2-3-4-12-13-14-0, has 4 interatomic bonds in the β plane $l_{0-14}$and two interatomic bonds l_{0-6} and l_{0-1} between parallel atomic planes. The length of the interatomic bond l_{0-14}, in the β plane, and the length of the interatomic bond l_{0-6}, between parallel atomic planes β and ɣ, have different lengths and therefore must have different forces of attraction. Taking into account the work [20], where the connection between the Poisson ratio and the change in the unit cell parameter $a_{Fe}$of iron was established, in the process of elastic deformation of the rod, it can be argued that the main elastic deformation of the cell occurs in the atomic planes, i.e. the elongation of the interatomic bond of the type l_{0-14} occurs. In fact, the Young's modulus E determined in the process of elastic deformation of the rod corresponds to the change in stress in the interatomic bonds of the type l_{0-14} (see Figure 3). Then the shear modulus G should correspond to the changes in the internal stress in the interatomic bonds of the type l_{0-6} (see Figure 3). Having established which interatomic bonds should correspond to the Young's modulus and the shear modulus, we distribute the electrons in the magnetic loops by introducing the coefficient χ denoting the ratio of the number of electrons in the magnetic loops, interatomic bonds, $l_{0-14}$and l_{0-6}as:

$$\chi = \frac{n_e^G}{n_e^E} = (1 - \frac{1}{2(1+\nu)}) = (1 - \frac{1}{2{,}54}) = 0{,}606 \approx 0{,}6 \quad (14)$$

The value of Poisson's ratio for iron is taken to be equal to $\nu = 0{,}27$. This value corresponds to the average value of the experimentally determined region of Poisson's ratio for iron $\nu = 0{,}231 - 0{,}31$ given in the reference book [11]. Considering that the total number of electrons $\sum n_e$ is the sum of all electrons in all "magnetic" loops.

$$\sum n_e = 4 * n_e^E + 2 * n_e^G = n_e^E * (4 + 2 * \chi) \quad (15)$$

We can calculate the number of electrons in a loop of the type l_{0-14} located in the atomic plane:

$$n_{e1} = \frac{\sum n_e}{(4+2\chi)} = \frac{5198}{4+2*0,6} = \frac{5198}{5,2} \approx 1000(things) \quad (16)$$

and, accordingly, the number of electrons in a loop of the type l_{0-6} that pulls together parallel atomic planes:

$$n_{e2} = 1000 * 0,6 = 600(things) \quad (17)$$

Now, to calculate the force of attraction f_i between electrons in the loops of type l_{0-14} and typel_{0-6}, we use the refined equation (2):

$$f_{ei} = \frac{e^2}{b_i^2} \quad (18)$$

Let us establish the distance b_i for each type of loop l_i by finding the total length of the loop for atoms located in one atomic plane. Let us consider Figure 5, which shows 3 possible variants of combining valence electrons into a "magnetic" loop. For clarity, the interatomic distance Δ is shown enlarged in relation to its true size.

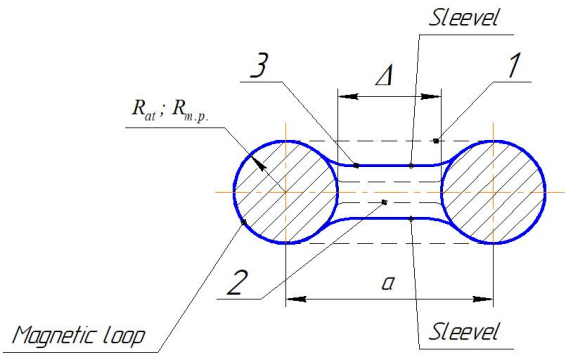

Fig. 5. The spatial arrangement of the "magnetic" loop.

When carefully considering the possible options for combining electrons into a loop, it is necessary to take into account that the selected volume of the loop (tube) (see Figure 2) is formed by rotation of electrons relative to the midline with a certain radius of electron revolution r_e relative to it. The circumferential velocity υ_ω creates pressure on the surface of the "tube" and therefore the loop sleeve, on the one hand, should repel, and on the other hand, the electrons in the loop sleeves should attract in accordance with Coulomb's law. It turns out that combination option 1 (Figure 5) does not take into account the attraction between electrons in parallel sleeves of one loop, and option 2 does not take into account the repulsion of the sleeves of the "magnetic" loop due to the pressure on the circumference of the tube. Therefore, it is logical to accept option 3 of the location of the "magnetic" loop in the space of two adjacent atoms. To calculate the length of the "magnetic" loop $l_{m.l}$, we assume that the radius of the "magnetic" loop $R_{m.l}$ enveloping the atom is equal to the radius of the atom $R_{m.l} = R_{at}$ itself. Let us assume that the chosen length of the "magnetic" loop, option 3, is the average length between the sum of the lengths of option 1 and option 2:

$$l_{m.l} = \frac{l_1+l_2}{2} = \frac{(2*\pi*R_{at}+2*a_{Fe}^1)+(2*\pi*R_{at}+2*\pi*R_{at}+2*\Delta_1)}{2} \quad (19)$$

Let's calculate the value of the average length of the "magnetic" loop for the type by taking the values $a_{Fe}^1 = 2,915 * 10^{-10}(m)$,$R_{at}^{Fe} = 1,26 * 10^{-10}(m)$ and $\Delta_1 = 0,395 * 10^{-10}(m)$:

$$l_{m.l} = (2 * 3,14 * 1,26 * 10^{-10} + 0,395 * 10^{-10}) + (3,14 * 1,26 * 10^{-10} + 2,915 * 10^{-10}) = 15,1792 * 10^{-10}(m) \quad (20)$$

Now we can calculate the value b_1 for a loop of type l_{0-14}. It is necessary to take into account that when the electrons of two neighboring atoms are combined into one common loop, the number of electrons in it will double and will be $2 * n_{e1}$.

$$b_1 = \frac{l_{m.l}}{2*n_{e1}} = \frac{15{,}1792*10^{-10}(m)}{2*1000} = 0{,}007589 * 10^{-10}(m) = 7{,}589 * 10^{-13}(m) \quad (21)$$

The force of attraction between electrons f_1 for a loop of type l_{0-14} according to (18) will be:

$$f_1 = \frac{(1{,}602*10^{-19}(C))^2}{(7{,}589*10^{-13}(m))^2} = \frac{2{,}566404*10^{-38}(C)^2}{57{,}5929*10^{-26}(m^2)} = 0{,}044561 * 10^{-12}(H) = 4{,}4561 * 10^{-14}(H) \quad (22)$$

To calculate the internal "zero" voltage in the loop $\sigma_{m.l}$, it is necessary to know the radius of electron circulation in the loop $r_{m.l}$. Assuming uniformity of electron motion both in the Compton wave and the motion of the electron wave, in the form of a "magnetic" loop, in the metal and knowing the value of the Compton wave length $\lambda_e = 2{,}43 * 10^{-12}(m)$, we find the radius of this wave:

$$R_{k.e} = \frac{\lambda_e}{2*\pi} = \frac{2{,}43*10^{-12}(m)}{2*3{,}14} = 0{,}38694 * 10^{-12}(m) \quad (23)$$

Let us assume that the radius of the magnetic loop corresponds to the radius of the Compton wave $R_{k.e} = r_{m.l} = 0{,}38694 * 10^{-12}(m)$ and has a constant value for all metals. Then the area of the loop $S_{m.l}$ will have a constant value (Const):

$$S_{m.l} = \pi * r_{m.l} = 3{,}14 * (0{,}38694 * 10^{-12}(m))^2 = 3{,}14 * 0{,}1497225 * 10^{-24}(m)^2 = 4{,}70129 * 10^{-25}(m)^2 \quad (24)$$

Now we have the opportunity to calculate the value of the internal "zero" stress $\sigma^E_{m.l}$ pulling the atoms together in the atomic plane. It is necessary to take into account that the loop has two arms and in each of them the force of attraction f_1 between the electrons acts, therefore, to overcome the forces of attraction, it is necessary to apply an external force $F \geq 2 * f_1$. The total stress in the two loops will have the value:

$$\sigma^E_{m.l} = \frac{2*f_1}{S_{m.l}} = \frac{2*4{,}4561*10^{-14}(H)}{4{,}70129*10^{-25}(m)^2} = \frac{8{,}9122*10^{-14}(H)}{4{,}70129*10^{-25}(m)^2} = 1{,}895 * 10^{11}(\frac{H}{m^2}) \approx 190(GPa) \quad (25)$$

The value of the "zero" voltage $\sigma^E_{m.l}$ of electrons in two arms of the "magnetic" loop for iron turned out to be equal to the lower limit of the value of Young's modulus $E = 190 \div 200(GPa)$ [11,13] obtained experimentally, which was assumed in advance given that the stress in the process of elastic deformation, in accordance with the deformation graphs, increases from the relative shift of atoms from the equilibrium position.

Now we will determine the theoretical value of the stress $\sigma^G_{m.l}$ in the loops between parallel atomic planes of the type l_{0-6} which should correspond to (be slightly less than) the value of the shear modulus G for iron. To do this, it is necessary to calculate the average value of the length of the "magnetic" loop $l^G_{m.l}$ taking into account the value of the gap between the atoms located between the parallel atomic planes α and β $\Delta_2 = 0{,}0044 * 10^{-10}(m)$ and the distance between the atoms themselves equal to:

$$a^{11}_{Fe} = \frac{a^1_{Fe}*\sqrt{3}}{2} = \frac{2{,}915*10^{-10}*1{,}732}{2} = 2{,}52439 * 10^{-10}(m) \quad (26)$$

Average value $l^G_{m.l}$ according to equation (19) will be as follows:

$$l^G_{m.l} = 3 * 3{,}14 * 1{,}26 * 10^{-10} + 2{,}52439 * 10^{-10} + 0{,}0044 * 10^{-10} = 14{,}39799 * 10^{-10}(m) \quad (27)$$

The area b^G_2 in the magnetic loop of type l_{0-6} after the unification of electrons will be:

$$b^G_2 = \frac{l^G_{m.l}}{2*n^G_e} = \frac{14{,}39799*10^{-10}(m)}{2*600} = 0{,}0119983 * 10^{-10}(m) = 1{,}19983 * 10^{-12}(m) \quad (28)$$

Accordingly, the force of attraction of electrons in the “magnetic” loop between parallel planes f^G_e will have the value:

$$f^G_e = \frac{e^2}{(b^G_2)^2} = \frac{2{,}566404*10^{-38}(C)^2}{1{,}43959*10^{-24}(m)^2} = 1{,}7827 * 10^{-14}(H) \quad (29)$$

Then the total value of the internal stress in the loop of type l_{0-6}, considering the two sleeves of the loop, will be:

$$\sigma_{m.l}^{G} = \frac{2*f_e^G}{S_{m.l}} = \frac{2*1,7827*10^{-14}(H)}{4,70128*10^{-25}(m)^2} = 0,7584 * 10^{11}(Pa) = 75,84(GPa) \quad (30)$$

The theoretical value of the "zero" stress in the loop between atomic planes in iron, without external deformation, is taken to be equal to $\sigma_{m.l}^{G} \approx 76(GPa)$. The experimentally established value $G = 81(GPa)$ [11,13] difference is only $\psi \approx 6\%$.

To test this theoretical method for calculating the value of Young's modulus E and the shear modulus G, we will establish the theoretical values of Young's modulus E and the shear modulus G for Cr (chromium).

Chromium data from the reference book [16]: atomic mass N_{Cr}- 51.9961 a.m.u.

$$m_{at}^{Cr} = 51,9961(a.m.u) * 1,660539066 * 10^{-27}\frac{kg}{a.m.u} = 86,32495 * 10^{-27}(kg) \quad (31)$$

$\rho_{Cr}(20°C) = 7190\frac{kg}{m^3}$; crystal lattice parameter $a_{Cr} = 2,885 * 10^{-10}(m)$; speed of sound in a rod $\upsilon_{st} = 5940(\frac{m}{s})$; longitudinal speed of sound $\upsilon_p = 6600(\frac{m}{s})$; atomic radius reference $R_{at}^{Cr} = 1,3 * 10^{-10}(m)$; empirical radius of an atom $R_{at}^{Cr} = 1,28 * 10^{-10}(m)$.

The mass of an atom under n. c. will be:

$$m_{at}^{Cr}(20°C) = 7190(\frac{kg}{m^3}) * \frac{1}{2} * (2,885 * 10^{-10}(m))^3 = 86,324 * 10^{-27}(kg) \quad (32)$$

The value of the mass of the chromium atom obtained in (32) is less than the value (31), which indicates the need to determine the parameter of the chromium crystal lattice under n. c. from condition (9). First, we calculate the theoretical radius of the chromium atom from the reference data of the parameter $a_{Cr} = 2,885 * 10^{-10}(m)$:

$$R_{at}^{Cr1} \leq \frac{a_{Cr}*\sqrt{3}}{4} \leq \frac{2,885*10^{-10}*1,732}{4} \leq 1,249 * 10^{-10}(m) \quad (33)$$

Now, knowing the three values of the radius of the chromium atom, we can find the average value as the quotient of dividing the three values - empirical, reference and calculated:

$$R_{at}^{Cr} = \frac{(1,28+1,249+1,3)*10^{-10}(m)}{3} \approx 1,275 * 10^{-10}(m) \quad (34)$$

Accordingly, having accepted the value of the radius of the chromium atom (34), we find a new value of the parameter a_{Cr} in accordance with the condition (9):

$$a_{Cr}^{1} \succ 4 * 1,2275 * 10^{-10}(m)/\sqrt{3} = 2,948 * 10^{-10}(m) \quad (35)$$

Accordingly, having accepted the value of the radius of the chromium atom (34), we find a new value of the parameter in accordance with the condition

Let us accept a new value $a_{Cr}^{1} = 2,95 * 10^{-10}(m)$. We will check the parameter of the chromium crystal lattice a_{Cr} based on a simplified model of sound transmission in metals between atoms by elastic interaction of atomic shells based on the equation:

$$\vartheta = l * \omega * \frac{1}{n} \quad (36)$$

where l is the length of the interatomic bond expressed through the lattice parameter a; ω is the frequency of atomic oscillation in the primitive volume of the crystal lattice; n is the number of interatomic bonds involved in the transmission of sound energy.

Equation (36) allowed us to calculate the theoretical values of the speed of sound for iron and copper, which coincided with high accuracy (95-100%) with the experimentally established values of the longitudinal, transverse and speed of sound in the rod for these materials. It should be noted that the model of elastic interaction of atomic shells is applicable only to the undeformed volume of the material under normal conditions, since it is a simplification of the model of interatomic interaction by magnetic loops. We find the natural frequency of oscillation of the chromium atom from the value of the speed of sound in the rod as:

$$\omega_{Cr} = \frac{v_{st}^{Cr}}{a_{Cr}^{1} * \frac{\sqrt{3}}{2}} = \frac{5940(\frac{m}{s})}{2{,}95 * 10^{-10}(m) * 0{,}866} = 2{,}32 * 10^{13}(Hz) \quad (37)$$

Accordingly, the theoretical value of the longitudinal speed of sound in chromium will be:

$$v_p^{Cr} = \omega_{Cr} * a_{Cr}^{1} * \frac{1}{n} = 2{,}32 * 10^{13}(Hz) * 2{,}95 * 10^{-10}(m) * \frac{1}{1} = 6850(\frac{m}{s}) \quad (38)$$

The obtained value (38) of the longitudinal speed of sound in chromium coincides with a sufficient degree of accuracy (difference $\psi = 4\%$) with the experimentally determined value of the speed of sound in chromium $v_0^{Cr} = 6600(\frac{m}{s})$ [13], which allows us to accept the value of the crystal lattice parameter of chromium as equal to $a_{Cr}^{1} = 2{,}95 * 10^{-10}(m)$.

Now we will calculate the mass of the chromium atom under n. c. from the new value a_{Cr}^{1}:

$$m_{at}^{Cr}(20°C) = 7190(\frac{kg}{m^3}) * \frac{1}{2} * (2{,}95 * 10^{-10}(m))^3 = 92{,}2921 * 10^{-27}(kg) \quad (39)$$

accordingly, the difference in the masses of atoms at different temperatures will be:

$$\Delta m_{at}^{Cr} = m_{at}^{Cr}(20^{\circ}C) - m_{at}^{Cr}(-273°C) = 92{,}2921 * 10^{-27}(kg) - 86{,}32495 * 10^{-27}(kg) = 5{,}967 * 10^{-27}(kg) \quad (40)$$

The additional number of electrons in a unit volume of a primitive cell of chromium $\sum n_e^{Cr}$ is:

$$\sum n_e^{Cr} = \frac{\Delta m_{at}^{Cr}}{m_e} = \frac{5{,}967 * 10^{-27}(kg)}{9{,}109 * 10^{-31}(kg)} = 6550(things) \quad (41)$$

The Poisson's ratio for chromium will be defined as:

$$\nu = 2(1 - \frac{l_{0-6}}{l_{0-14}}) = 2(1 - \frac{\sqrt{3}}{2}) = 2 - 1{,}732 \approx 0{,}27 \quad (42)$$

The value of the Poisson ratio of chromium coincides with the value of the Poisson ratio of iron, which is associated with the identical structure of metals, which have the same type of primitive cell of the crystal lattice.

$$\chi_{Cr} = \frac{n_e^G}{n_e^E} = (1 - \frac{1}{2(1+\nu)}) = (1 - \frac{1}{2{,}54}) = 0{,}606 \quad (43)$$

Accordingly:

$$n_{e1}^E = \frac{\sum n_e}{(4+2\chi)} = \frac{6550}{4+2*0{,}606} = \frac{6550}{5{,}212} \approx 1256(things) \quad (44)$$

$$n_{e2}^G = 1256 * 0{,}606 \approx 760(things) \quad (45)$$

$$\Delta_E = a_{Cr}^{1} - 2 * R_{at}^{Cr} = (2{,}95 - 2 * 1{,}275) * 10^{-10}(m) = 0{,}4 * 10^{-10}(m) \quad (46)$$

$$\Delta_G = a_{Cr}^{1} * \frac{\sqrt{3}}{2} - 2 * R_{at}^{Cr} = (2{,}554 - 2 * 1{,}275) * 10^{-10}(m) = 0{,}004 * 10^{-10}(m) \quad (47)$$

The average length of the "magnetic" loop of type l_{0-14} (corresponding to the values of Young's modulus E) for chromium will have a value:

$$l_{0-14}^{Cr} = 3 * \pi * R_{at}^{Cr} + a_{Cr}^{1} + \Delta_E = 3 * 3{,}14 * 1{,}275 * 10^{-10}(m) + 2{,}95 * 10^{-10}(m) + 0{,}4 * 10^{-10}(m) = 15{,}3605 * 10^{-10}(m) \quad (48)$$

The distance between electrons b_E^{Cr} in a "magnetic" loop of the type l_{0-14} will have a value equal to:

$$b_E^{Cr} = \frac{l_{0-14}^{Cr}}{2 * n_{e1}^E} = \frac{15{,}3605 * 10^{-10}(m)}{2512} = 0{,}006114 * 10^{-10}(m) = 6{,}114 * 10^{-13}(m) \quad (49)$$

The force of attraction between two adjacent electrons in a "magnetic" loop l_{0-14}will be:

$$f_{e1}^{Cr} = \frac{(1{,}602 * 10^{-19}(C))^2}{(6{,}114 * 10^{-13}(m))^2} = \frac{2{,}566404 * 10^{-38}(C^2)}{37{,}3321 * 10^{-26}(m^2)} = 0{,}0687 * 10^{-12}(H) = 6{,}87 * 10^{-14}(H) \quad (50)$$

The internal stress in the “magnetic” loop l_{0-14} for chromium, given the constant value of the Compton wave area – $S_{m.l}$, under normal conditions, will have a theoretical value equal to:

$$\sigma_{Cr}^{E0} = \frac{2 * f_{e1}^{Cr}}{S_{m.l}} = \frac{2 * 6{,}87^{-14}H}{4{,}70129 * 10^{-25}{}_M{}^2} = \frac{13{,}74 * 10^{-14}(H)}{4{,}70129 * 10^{-25}(m^2)} = 2{,}9226 * 10^{11}\left(\frac{H}{m^2}\right) \approx 292(GPa) \quad (51)$$

The obtained theoretical value of internal stress (51) is slightly lower than the experimentally established value of Young's modulus E of chromium – 300 GPa [12,14] in the region of elastic deformation.

In the same way, we determine the shear modulus G of chromium:

$$l_{0-6}^{Cr} = 3 * \pi * R_{at}^{Cr} + a_{Cr}^{1} * \frac{\sqrt{3}}{2} + \Delta_G = 12{,}0105 * 10^{-10}(m) + 2{,}5547 * 10^{-10}(m) + 0{,}004 * 10^{-10}(m) = 14{,}5692 * 10^{-10}(m) \quad (52)$$

$$b_G^{Cr} = \frac{l_{0-14}^{Cr}}{2 * n_{e2}^{G}} = \frac{14{,}5692 * 10^{-10}(m)}{2 * 760} = 0{,}009585 * 10^{-10}(m) = 9{,}585 * 10^{-13}(m) \quad (53)$$

$$f_{e2}^{Cr} = \frac{(1{,}602 * 10^{-19}(C))^2}{(9.585 * 10^{-13}(m))^2} = \frac{2{,}566404 * 10^{-38}(C^2)}{91{,}8722 * 10^{-26}(m^2)} = 0{,}027934 * 10^{-12}(H) = 2{,}79 * 10^{-14}(H) \quad (54)$$

$$\sigma_{Cr}^{G0} = \frac{2 * f_{e2}^{Cr}}{S_{m.l}} = \frac{2 * 2{,}79^{-14} H}{4{,}70129 * 10^{-25}{}_{M}{}^{2}} = \frac{5{,}58 * 10^{-14}(H)}{4{,}70129 * 10^{-25}(m^2)} = 1{,}18 * 10^{11}(\frac{H}{m^2}) = 118(GPa) \quad (55)$$

The experimental value of the shear modulus of chromium varies within the limits $G \approx 110 - 125(GPa)$ depending on the source. Thus, the calculated theoretical value of the shear modulus of chromium (55) coincides with the arithmetic mean value of the shear modulus of chromium determined in experiments. The high accuracy of the coincidence of the theoretical values of Young's modulus and the shear modulus for iron and chromium with the experimental values allows us to accept the new model of interatomic interaction, the contraction of atoms by "magnetic" loops, as a basis for calculating other metals. Below is Table 1 for a number of metals that were theoretically calculated using equation (3) with refinements of the crystal lattice parameters for them.

Table 1. Theoretical values of the shear modulus of metals calculated using a new model of interatomic interactions.

	E_{teor} ГПа	E_{exper} ГПа	G_{teor} ГПа	G_{exper} ГПа	$L_{m.l}^{E} * 10^{-10}$	$L_{m.l}^{G} * 10^{-10}$	$R_{at}^{teor} * 10^{-10}$	$R_{at} * 10^{-10}$	$a_{teor} * 10^{-10}$	$a * 10^{-10}$	$m_{at}^{nor.con} * 10^{-27}$	*Crystal lattice*
Fe	190	190-200	75.85	81	15.1792	14.3979	1.26	1.26	2.91	2.866	97.4676	bcc
Cr	292	300-330	118	110-125	15.3605	14.5692	1.275	1.30	2.95	2.885	92.2921	bcc
W	362.8	350-400	145	133-150	16.5654	15.6702	1.37	1.41	h-3.17 a-3.2	3.16	312.425	bcc/?
Ba	14.4	13	6	4.9	25.662	24.2763	2.1	2.22	5.02	5.02	2.20412	bcc
Cu	130	110-130	43.5	40-50	16.8026	14.6656	1.28	1.28	3.655	3.615	108.8847	fcc
Pb	166.23	162	54.6	56.2	22.564	19.6483	1.7	1.75	4.975	4.95	349.132	fcc
Ni	19.5	20.2	6.25	7.7	16.276	14.2031	1.24	1.24	3.54	3.524	98.569	fcc
Al	70.26	68.5	23.19	24.5	18.648	16.2278	1.4	1.43	4.13	4.050	47.531	fcc
Mg	45.1	41-45	16.75	16-16.5	22.207	18.278	1.6	1.6	a-3.203 c-5.2	a-3.202 c-5.2	42.969	hcl
V	126.5	126.5 - 139.4	50.3	47	15.79	14.9666	1.3	1.34	3.072	3.024	88.56759	bcc
Mo	325	336.3	129	122	16.447	15.5871	1.35	1.39	h-3.142 a-3.216	3.147	159.7175	bcc/?

In some cases, the refinement of the crystal lattice parameter based on inequality (9) leads to the refinement of the crystal lattice geometry. For example, tungsten and molybdenum most likely belong to the rhombic body-centered crystal lattice.

Considering the high accuracy of the coincidence of the theoretical values of the Young's modulus and the shear modulus for metals, we will apply this calculation model to alloys.

For the theoretical calculation of the alloy, we will take steel 08Kh17T with an established theoretical value of Young's modulus equal to 206 GPa [11]. The composition of this steel, in percentage content of substances, consists of 80.2% iron, 17% chromium and 2.8% is carbon (<0.08), silicon (<0.8), manganese (<0.8), phosphorus (<0.035), molybdenum (<0.3) and other elements. It is necessary to understand that the distribution of Cr in the volume of iron is chaotic, but on one line in the atomic plane (chain of atoms) there should be 17% of chromium atoms. Thus, in a chain of 100 consecutively located alloy atoms there should be 17 chromium atoms. The atoms can be located in any sequence, for example, as shown in Figure 6

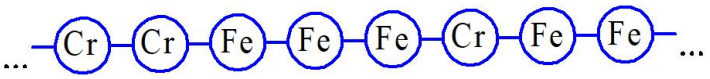

Fig. 6. Atomic distribution of chromium in steel 08Kh17T: a theoretical model.

To consider this alloy, we introduce the condition that the energy of the interatomic bond, the energy of the "magnetic" loop $E_{m.l}$, any type of bond in the alloy $Cr-Cr, Fe-Fe$ - or $Cr-Fe$ is a constant value:

$$E_{m.l.} = Const \tag{56}$$

This condition (56) can be fulfilled only under the condition that the mass (quantity) of electrons in any loop of any type of connection $Cr-Cr, Fe-Fe$ and $Cr-Fe$ is a constant value, that is, the electrons of chromium and iron are actually socialized with a redistribution of their number in the "magnetic" loops to one value:

$$N_{Cr-Fe} * m_e = Const \tag{57}$$

Taking into account conditions (56) and (57), we will carry out a theoretical calculation of the value of Young's modulus for steel 08X17T. The average value of the loop length l_{Cr-Fe} for an arbitrary arrangement of atoms (see Figure 6) can be determined as:

$$l_{Cr-Fe} = \frac{(81*l_E^{Fe}+17*l_E^{Cr})}{100} \tag{58}$$

The theoretical value of the average loop length will be:

$$l_{Cr-Fe} = \frac{81 * 15{,}1792 * 10^{-10}(m) + 17 * 15{,}3605 * 10^{-10}(m)}{100} = 12{,}295152 * 10^{-10}(m) + 2{,}611285 * 10^{-10}(m) = 14{,}906435 * 10^{-10}(m) \tag{59}$$

The number of electrons per loop is defined as:

$$n_E^{Cr-Fe} = \frac{81*n_E^{Fe}+17*n_E^{Cr}}{100} = 0{,}81 * 1000 + 0{,}17 * 1256 = 810 + 213{,}54 \approx 1024(things) \tag{60}$$

Then the distance b_E^{Cr-Fe} between electrons in the loop, taking into account the doubling of electrons, will be:

$$b_E^{Cr-Fe} = \frac{l_{Cr-Fe}}{2*n_E^{Cr-Fe}} = \frac{14{,}906435*10^{-10}(m)}{2*1024} = 0{,}0072785 * 10^{-10}(m) = 7{,}2785 * 10^{-13}(m) \tag{61}$$

The attractive force between electrons in the loop f_e^{Cr-Fe} will be equal to:

$$f_e^{Cr-Fe} = \frac{e^2}{(b_E^{Cr-Fe})^2} = \frac{2{,}566404*10^{-38}(C^2)}{(7{,}2785*10^{-13}(m))^2} = 4{,}8444 * 10^{-14}(H) \tag{62}$$

And accordingly, taking into account that the area of the loop under normal conditions $S_{m.l}$ in any material should not change, the internal stress holding the atoms relative to each other will have a value equal to:

$$\sigma_0^{Cr-Fe} = \frac{2*f_e^{Cr-Fe}}{S_e} = \frac{2*4{,}8444*10^{-14}(H)}{4{,}70129*10^{-25}(m^2)} = 2{,}06088 * 10^{11}(Pa) \approx 206{,}1(GPa) \tag{63}$$

The theoretical value of the "zero" stress σ_0^{Cr-Fe} holding atoms in the alloy (steel) 08X17T, based on a new model of interatomic interaction - "magnetic" loops, almost 100% coincides with the experimentally determined value of Young's modulus for this alloy. The table below shows calculations for some alloys of magnesium, aluminum, lead and copper.

The experimental values of Young's modulus for these alloys are taken from [14]. It is evident from the table that the theoretical values of Young's modulus for the alloys are very close to, or practically coincide with, the experimentally established values of Young's modulus for these materials.

Table 2. Theoretical vs. experimental Young's modulus values for various alloys based on the "magnetic" loops model.

	E_{teor} GPa	$E_{exp\,er}$ GPa	$L_{m.l}^{E} * 10^{-10}$
Mg_2Cu	58.5	62.5	20.96004
Mg_2Pb	83.69	69.2	22.3856
$Mg_{17}Al_{12}$	52.45	57.6	21.03984
$AlCu$	69.77	70	18.3839

4 Conclusion

The proposed method for calculating the internal - "zero" stress in metals and their alloys under n. c. based on a new expression (equation):

$$\sigma_0 = \frac{e^2}{b_i^2 * S_{m.p}}$$

where b_i- distance between electrons in "magnetic" loops; $S_{m.p}$- the area of a magnetic loop, under normal conditions has a constant value for metals.

The method allows to calculate Young's modulus and shear modulus G for the same metal and alloys based on this metal, which became possible due to the new concept of interatomic bond as a "magnetic" (electromagnetic) loop, pulling together neighboring atoms, both in the atomic plane and neighboring parallel atomic planes. This model of pulling together atoms by a "magnetic" (electromagnetic) loop meets the criteria for evaluating proposed by Lenz, since the model for theoretically calculating Young's modulus and shear modulus has a simple explanation that is complete and exhaustive and is based on a single formula. At the same time, other phenomena occurring in metals under elastic deformation are also explained based on the new model of interatomic interaction - cooling, heating and changes in the speed of ultrasound based on changes occurring in the loop itself [2]. Thus, the new Physical model of interatomic interaction is universal for considering most physical processes occurring in metals under the influence of temperature and deformation. The high degree of agreement between the theoretical values of the Young's modulus E and the shear modulus G with the experimentally established values confirms the proposed assumption about the absorption of external energy in the form of electron energy quanta in the material by "magnetic" loops, which allows us to further consider the process of heat capacity and heat transfer based on the propagation of energy through loops, as well as the assumption that the Compton wave retains its dimensions in the crystal lattice of the material.

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