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ON THE MICROSCOPIC NATURE OF THE YOUNG MODULUS

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On introducing the Van der Waals forces and Kittel mechanism of coupling into consideration, a physical approach to analytical computation of the Young modulus E has been outlined. By using a numerical analysis, a nontrivial behavior of the dependence of E on the atomic mass of an element has been predicted.

Within the framework of the continuum approach of elasticity theory, the Young modulus E is considered as a certain phenomenological parameter [1–3], the values of which can be found experimentally by the method of longitudinal extension of thin rods.

The object of the present investigation is an analysis of the function $E(A)$ proceeding from certain purely physical assumptions.

If a metal rod is being torn asunder, then, as numerous experiments show (the references are not listed because of their exceedingly great number), the value of E will not depend on the rod length l when it decreases to as low as the interatomic distance. The latter clearly points only to the fact that the nature of the break is microscopic and therefore the breaking force must be closely related to purely microscopic interactions.

By taking into consideration the dimensionality of the Young modulus, viz., dyn/cm^2 or erg/cm^3, which is the energy of the unit volume of a body, it becomes evident that the quantity E correlates only with the internal potential energy attributable to the interaction of the atoms located at a certain distance a from one another. From dimensionality considerations it follows that

$$E = \frac{|\overline{U}|}{a^3} . \tag{1}$$

Physically, the role of the potential energy may belong both to the Van der Waals (VW) interaction attributable to the purely electromagnetic nature of the coupling and the Ruderman–Kittel (RK) one, which in metals plays the role of the Heisenberg exchange interaction. But in the general case, by virtue of the additivity of potential energies we write $U = U_{\mathrm{VW}} + U_{\mathrm{RK}} + U_{\mathrm{H}}$, where the last term accounts for the purely magnetic nature of exchange interaction inherent in magnets (e.g., iron) and represents, as is known [4], the Heisenberg spin–spin interaction of the outer shells of atoms. A more detailed discussion of the contribution of U_{RK} follows below.

Since, according to [5], $\overline{U}_{\mathrm{VW}} = \dfrac{23\hbar c}{4\pi r^7}\alpha_1\alpha_2$, assuming that $r = a$ we obtain from Eq. (1) the following formula to calculate the elasticity modulus:

$$E = \frac{23\hbar c}{4\pi a^{10}}\alpha_1\alpha_2 . \tag{2}$$

By virtue of the definition of polarizability at $\alpha_1 = \alpha_2 = \xi a_{\mathrm{B}}^3$, where ξ depends on the atomic mass A of an element in the Mendeleev table, whereas $a_{\mathrm{B}} = \hbar^2/(me^2) = 0.5\cdot 10^{-8}$ cm, and from Eq. (2) we find that

$$E = \frac{23\hbar c}{4\pi a^4}\left(\frac{a_{\mathrm{B}}}{a}\right)^6 \xi^2(A) . \tag{3}$$

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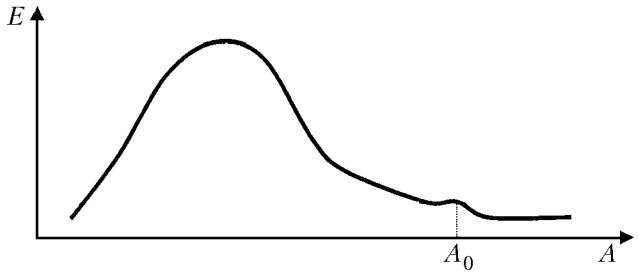

Fig. 1. Schematic behavior of the Young modulus depending on the atomic mass A of an element from the Mendeleev table of elements.

Selecting the distance $a = a_0 = 2.36 \cdot 10^{-8}$ cm and assuming that $\xi = 1$, at $\hbar = 10^{-27}$ erg·sec and $c = 3 \cdot 10^{10}$ cm/sec, we obtain

$$E = E_0 = 0.16 \cdot 10^{11} \text{ Pa} . \tag{4}$$

As is seen from Table 1, the given value corresponds, with an acceptable accuracy, to the Young modulus for lead and is taken as a standard. We also take the value of a_0 as a standard. For further convenience, we rewrite Eq. (3) in the form

$$E = E_0 \Phi (A) , \tag{5}$$

where $E_0 = \dfrac{23\hbar c}{4\pi a_0^4} = 0.16 \cdot 10^{11}$ Pa, whereas the function $\Phi(A) = \left(\dfrac{a_B}{a_0}\right)^6 \xi^2(A)$ needs determination.

The numerical analysis based on the method of nonlinear correlation has shown that to obtain a satisfactory agreement of E with the values for the remaining elements of the table, the form of the function $\Phi(A)$ should be as follows:

$$\Phi (A) = 10^{-4} S (A) A^{3.8} \exp (-A/10) (4.39 \cdot 10^{-3} A^3 - 0.75A^2 + 40.5A - 609.75) , \tag{6}$$

where $S(A) = 0.1[1 + 9\theta(A - A_0)]$ is the step function in which $\theta(x)$ is the Heaviside function determined according the standard rule

$$\theta (x) = \begin{cases} 1 , & \text{if } x > 0 ; \\ 0 , & \text{if } x \le 0 , \end{cases} \tag{7}$$

and the atomic mass A_0 plays the role of the parameter the value of which is unknown and therefore we may only state that A_0 is of the order of 100. It is quite probable that the role of the corresponding element with the atomic number Z_0 belongs to tin; however, this assumption needs experimental verification. A nontrivial fact may be that such a metal exists in nature but has not yet been found.

Dependence (6) is illustrated in Fig. 1. It is seen that at $A = A_0$ a local maximum of the function $\Phi(A)$ is reached. It can be easily verified by direct substitution that for tin with $A \approx 118$ we obtain from Eq. (5), subject to Eqs. (4) and (6), the value

$$E = 0.873 \cdot 10^{11} \text{ Pa} , \tag{8}$$

which, as is seen from Table 1, is close to the value taken by us from the reference data of [6]. All the remaining values of the Young modulus (it can also be verified easily with the aid of Eqs. (5) and (6)) given in Table 1 are described by Eq. (6) within 3–7%.

In order to predict the values of E for other metals, we consider, as an example, five elements: Au (A = 119), Pt (A = 195), W (A = 184), Ag (A = 108), and Ti (A = 47.9). According to Eq. (6) we have

TABLE 1. Values of the Young Modulus

A	27 (Al)	56 (Fe)	64 (Cu)	118 (Sn)	207 (Pb)
$E\cdot 10^{-11}$, Pa	0.7	2.1	1.3	0.9	0.16
$E\cdot 10^{-11}$, Pa; calculation by Eq. (5)	0.69	2.04	1.208	0.873	0.16

$$E_{\mathrm{Au}} = 0.293\cdot 10^{11}\ \mathrm{Pa}\,,$$

$$E_{\mathrm{Pt}} = 0.329\cdot 10^{11}\ \mathrm{Pa}\,,$$

$$E_{\mathrm{W}} = 0.614\cdot 10^{11}\ \mathrm{Pa}\,,$$

$$E_{\mathrm{Ag}} = 0.980\cdot 10^{11}\ \mathrm{Pa}\,, \tag{9}$$

$$E_{\mathrm{Ti}} = 3.01\cdot 10^{11}\ \mathrm{Pa}\,.$$

The above numerical values are in satisfactory agreement with [7].

Thus, with the aid of the proposed approach and using a numerical analysis, it has been proved that the Young modulus can be entirely determined by one parameter, viz., by the atomic mass of the metal considered. Attention should also be paid to the following important fact. In metals there is such a type of interaction between polarized (in a magnetic sense) atoms as the Ruderman–Kittel exchange coupling U_{RK} [8] attributable to the spin character of atoms with partially open *d*- or *f*-shells. It manifests itself due to the exchange by conduction electrons among these atoms because of the fact that the electrons transfer interaction as a faster subsystem.

But when we speak of metals, along with the Van der Waals interaction one should also take into account U_{RK}. However, since, in order of magnitude [8], $U_{\mathrm{RK}} \sim J_{s-d}^2/\varepsilon_{\mathrm{F}}$, where J_{s-d} is the energy of exchange coupling and ε_{F} is the Fermi energy, and it is possible to consider that $U_{\mathrm{RK}} \approx 10^{-13}$ erg, the additive contribution to E by U_{RK} will be on the order of $U_{\mathrm{RK}}/a^3 \sim 10^8$ Pa, which is much less than the Van der Waals contribution U_{VW}, and therefore we ignore U_{RK}.

CONCLUSIONS

1. The microscopic nature of the coefficient of longitudinal deformation has been analyzed.
2. An approximating formula describing the dependence of E on the atomic mass for a metal of arbitrary type has been suggested.
3. Due to the approach outlined (Eqs. (6) and (7)), a number of values of E have been calculated (see Eq. (9)).
4. Attention is drawn to the Young modulus jump beginning from a certain atomic mass A_0.

NOTATION

A, atomic mass of an element in the Mendeleev table of elements; A_0, phenomenological parameter; a, interatomic distance; a_0, standard interatomic distance; a_{B}, Bohr radius; c, speed of light in a vacuum; e, electron charge; E, Young modulus; E_0, standard Young modulus; $\hbar$, Planck constant; J_{s-d}, energy of *s*-*d*-exchange interaction; m, electron mass; U, potential energy; α, coefficient of atom polarization; Φ, approximating function; $\theta(x)$, Heaviside function; ξ, numerical factor. Subscripts: VW, RK, and H, Van der Waals, Ruderman–Kittel, and Heisenberg interactions.

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