CALCULATION OF MECHANICAL STRENGTH OF CRYSTALLINE LATTICES OF IRON, MOLYBDENUM, AND TUNGSTEN

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Semiempirical tensor equations of state were obtained for iron, molybdenum, and tungsten and used to examine the mechanical properties of their crystalline lattices under conditions of a complex system of stresses. The most hazardous systems of stresses were distinguished, and stresses and deformations were calculated. The obtained values of strength are in good agreement with the existing empirical data.

The systematic experimental study of mechanical properties of perfect crystals with body-centered cubic lattice has led to gradual accumulation of data which require definite theoretical generalization. However, at present, as far as we are aware, only roughly qualitative estimations of the behavior of ideal crystalline lattices under conditions of simple systems of stresses are available in the literature, while the greatest interest lies in the investigation of the behavior of lattices under conditions of complex systems of stresses, corresponding to the conditions of experiment. Therefore, it is of vital interest to examine, possibly completely and sequentially, the problem of mechanical properties of the ideal crystalline lattices, and particularly, of the character and parameters of mechanical destruction.

In [1] we have developed the scheme of studying the behavior of crystalline lattices under conditions of arbitrary systems of stresses. The key point in that study is the function of the energy of metallic bond. The statistical approximation of the quantum theory of the solid body allows to find the function of the energy of metallic bond in the form

\[ U = U_e + U_v + U_p, \]  

(1)

where \( U_e \) is energy of electrostatic interaction of the system of lattice-forming point-like positive ions with the uniformly distributed negative compensating charge; \( U_v \) is associated with the presence of free electrons in the metal, and depends only on the volume of the elementary cell \( v \); \( U_p \) is associated with the overlap of electron shells of ions, and leads to the occurrence of forces of the conjugate interaction type. That model and inferences following from it remain in good agreement with quantum mechanical calculations.

In [2], on the basis of the function of binding energy (1), the mechanical properties of alkali metals were investigated; it was assumed that the pairing interaction is small and the last term in (1) can be disregarded, which makes it possible to write the binding energy function, as well as the resulting from it equations of state, in the nonparametric form.

In passing to iron, molybdenum, and tungsten, the necessity arises of taking into account the pairing interaction. The equation (1) gives the possibility of carrying out the estimation of the contribution of that interaction by using experimental values for elastic moduli. In [3] it was shown that if the contribution of pairing interaction in the binding energy function is disregarded then between the elastic moduli of metals

having a body-centered cubic lattice the relation exists

$$\frac{C_{11} - C_{12}}{C_{44}} = 0.223.$$  

It is obvious that deviation of the experimental value of relation \((C_{11} - C_{12})/C_{44}\) from 0.223 will characterize the contribution of pairing interaction. For iron, molybdenum, and tungsten that deviation has corresponding values 0.605; 2.36; and 1.79; i.e. the contribution of pairing overlap in these metals is quite large and it is absolutely necessary to take it into account. The subsequent calculation in that case meets with insuperable difficulties, and a necessity arises for constructing the semiempirical function of binding energy and for obtaining on its basis the tensor equations of state. In [4] we have obtained the tensor equations of state for cubic face-centered lattices in the form

$$X_{ik} = -C_{44} \sum_{n=1}^{6} \left[ \frac{[Ik]_{n+2}}{S_{n+2}^{(l)}} \right] b_{n} + a_{n} \right] \rho^{2n+1},$$

(2)

where \(X_{ik}\) are components of stress tensor, \(C_{44}\) is elastic modulus, \(\rho = \rho_0/\rho\) is density of material, quantities \(l_{n+2}\) are sums along the lattice points depending only on the elementary cell, \(S_{n+2}^{(l)}\) is the value of \([Ik]_{n+2}\) for the cubic lattice, \(a_{n}\) and \(b_{n}\) \((b_2 = b_3 = b_5 = 0)\), are dimensionless parameters, determined with the use of experimental values of elastic moduli of constant lattice, and of empirical equation of state for hydrostatic compression. In the case of metals with body-centered cubic lattice, considered in this study, we arrive at similar equations of state; parameters \(a_{n}\) and \(b_{n}\) are presented in Table 1.

The tensor equations of state (2) make it possible to calculate the values of parameters of lattice deformation for the given system of stresses, and the conditions of thermodynamical stability [5], to find their critical values, and, consequently, values of stresses leading to the destruction of the lattice. These critical values form, in the space of stress tensor components, a surface representing the diagram of the anisotropic strength of the lattice. General analysis of properties of that surface, based on the symmetry

![Fig. 1](image1.png)

![Fig. 2](image2.png)