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# Determination of Young's modulus of metal-based composites with cubic lattice

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A quantum-mechanical approach in the density functional theory is proposed for calculation of elastic modulus of composite materials. The modulus of elasticity is the ratio of the changes in the total energy and volume of the crystal lattice when the crystal is deformed in a certain crystallographic direction. The elastic moduli of Ni, Cu and composites based on them have been calculated in the [100] and [110] directions. The results are in good agreement with the experimental data obtained by bending the substrate and measuring the mechanical stress arising in the metal film deposited on the substrate.

**Keywords**: modulus of elasticity, quantum-mechanical approach, total energy, density functional theory, composite electrolytic coatings, ultradispersed diamond, pulsed current.

**Визначення модуля Юнга композитів на основі металів із кубічною граткою.** *В.В. Титаренко*

Запропоновано квантово-механічний підхід у рамках теорії функціоналу густини для розрахунку модуля пружності композиційних матеріалів. Модуль пружності визначається як відношення зміни повної енергії кристалічної ґратки і зміни її об'єму при деформації кристала в певному кристалографічному напрямку. Розраховані значення модулів пружності Ni, Cu та композитів на їх основі в [100] та [110] напрямках. Результати розрахунків добре узгоджуються з експериментальними даними, отриманими методом вигину підкладки та вимірювання механічної напруги, що виникає в нанесеній на підкладку металевій плівці.

## *1. Introduction*

One of the most important areas of scientific and technological progress is related to improving the efficiency of composite materials; this makes the task of determining the elastic properties of crystalline materials one of the fundamental problems of the physics of strength and plasticity. This task can be solved, in particular, by modelling and calculating the elastic properties of metals, and the values determined in this way, for example, the elastic modulus, are necessary for solving many problems in strength physics, in particular, the Griffiths problem [1]. Moreover, existing methods for calculating Young's modulus are limited to certain average values and do not allow determining Young's moduli for different crystallographic directions [hkl]. There are many works on the theoretical determination of Young's modulus of mono- and polycrystalline materials, but this problem cannot yet be considered completely solved, especially with regard to studies of the elastic properties of metal-based composite materials.

The strength properties of any crystalline material depend primarily on the forces of intermolecular or interatomic interaction, which are commensurate with the elastic modulus. This is especially noticeable in single-crystal samples, the fracture of which occurs only along certain crystallographic planes and is associated with the breaking of bonds in the crystal lattice. At the same time, for polycrystalline materials, fracture can occur along interphase boundaries.

In all known methods for calculating Young's modulus, the main task is to determine the forces or binding energy between neighbouring atoms, ions, or molecules, depending on the type of crystal structure. For metallic materials, this is the interaction of ions. In a number of methods for calculating Young's modulus, only Coulomb interaction is taken into account [2], which, in our opinion, is not an accurate enough approximation, since it does not fully describe the interaction energy in the crystal lattice. In [3], the elastic modulus of a crystal was determined by replacing the binding energy of atoms with the sum of the heat of fusion and the heat of vaporisation, i.e., the energy of sublimation. A number of works use a quantum mechanical approach to find the energy. Thus, in [4], the Hartree-Fock self-consistent field approximation is applied, which in some cases gives good results but does not take into account the effects of electron correlation. At the same time, in [5], the electron correlation is taken into account by a functional that does not contain the electron density gradient, and no correction is made for the final size of the basis set used in calculating the total energies and binding energies, which, in turn, is not optimised over the entire configuration space and contains different parameter values for its different regions.

Thus, despite a significant number of approaches to determining the elastic characteristics of crystalline materials, the question of developing a universal method that allows calculating Young's moduli for various crystallographic directions with sufficient accuracy remains open and requires further research.

This paper presents the results of theoretical calculations of Young's modulus of FCC metals Ni and Cu and composites based on them, carried out within the framework of a quantum mechanical approach that takes into account the effect of electron correlation, i.e., static and dynamic interelectronic interactions in crystals. The calculated data were compared with experimental values measured by the substrate bending method before and after the deposition of the metal film.

## 2. Calculation of the elastic modulus

In this work, Young's modulus $E$ in a given crystallographic direction is defined as the ratio of the change in the total energy $\Delta W_{\mathrm{hkl}}$ of the crystal lattice to the change in its volume $\Delta V_{\mathrm{hkl}}$, when the crystal is deformed in the same direction:

$$E_{hkl} = \frac{\Delta W_{hkl}}{\Delta V_{hkl}} . \quad (1)$$

The change in the total energy of the crystal lattice is understood as the difference between the total energies of the crystal in the unstrained ($W_{total}$) and strained in the [hkl] direction states ($W_{hkl}$), i.e.:

$$\Delta W_{hkl} = \left| W_{total} - W_{hkl} \right| . \quad (2)$$

To calculate these energies, we propose to use a quantum mechanical approach within the framework of density functional theory (DFT), which takes into account the effect of electron correlation. The use of DFT provides sufficiently high accuracy of calculations with moderate requirements for computational resources.

To determine the energy $W_{total}$, we constructed a crystal lattice, which was then expanded in three directions, thereby creating a crystal with a volume $V$. The tensile strain of the crystal was simulated for various crystallographic directions, for each of which the geometric configuration with a volume $V_{hkl}$ was determined. According to the literature [6], elastic strain in metals should not exceed tenths of a percent, therefore, the crystal strain in the calculations was set to a 0.1% tensile strain in the selected crystallographic directions, while the other parameters of the crystal lattice remained unchanged.

The total energy $W_{total}$ or $W_{hkl}$ in the density functional theory is defined as:

$$W = U - \tfrac{1}{2} \sum_{i=1}^{N_{filled}} \int \varphi_i^*(r) \nabla^2 \varphi_i(r) dr - \quad (3)$$

$$-\sum_K Z_K \int \frac{\rho(r)}{\left| r - R_K \right|} dr + \frac{1}{2} \iint \frac{\rho(r)\rho(r')}{\left| r - r' \right|} dr dr' + ,$$

$$+E_{XC}\left[\rho\right]$$

where $Z_k$ and $R_k$ are the charge and the spatial coordinates of the fixed nucleus with the number $k$, respectively.

The reductive form of expression (3) is as follows:

$$\begin{aligned} W = U + T_S \left\{ \varphi_i(r) \right\}_{i=1}^{N_{filled}} + \\ + V_{ne}\left[\rho\right] + J\left[\rho\right] + E_{XC}\left[\rho\right] \end{aligned} . \quad (4)$$

The electron density ρ is defined as:

$$\rho(r) = \sum_{i=1}^{N_{filled}} \left| \varphi_i(r) \right|^2 , \quad (5)$$

where $\varphi_i(r)$ is the one-electron (molecular) Kohn-Sham orbital.

In the right-hand side of equation (4), the first term $U$ represents the potential energy of interaction between nuclei, the second term $T_S$ describes the electron kinetic energy, the third term $V_{ne}$ denotes the attraction of electrons to nuclei, the fourth term $J$ represents the classical interelectronic repulsion, and the last term $E_{xc}$ is the exchange-correlation functional, which includes static electron correlation.

The development of DFT led to the emergence of the generalised gradient approximation (GGA) [7], in which the exchange-correlation functional, including the absolute value of the density gradient, determines not only the electron density but also its inhomogeneity:

$$E_{XC}^{GGA} = \int \varepsilon_{XC}^{GGA}\left[\rho_\alpha(r),\left|\nabla\rho_\alpha(r)\right|;\rho_\beta(r),\left|\nabla\rho_\beta(r)\right|dr\right], \quad (6)$$

where $\rho_\alpha$ and $\rho_\beta$ are the densities of α- and β-electrons, respectively, and $\varepsilon_{xc}^{GGA}$ is the energy density per electron.

Hybrid functionals, which represent equations (6) as a linear combination of exchange and correlation functionals with different weighting factors determined empirically, provide a balance between the elimination of self-interaction and taking into account non-dynamic correlation.

One of them is the hybrid Becke-Perdew functional BP86, which consists of the exchange Slater-type Becke functional B [7], including the density gradient, and the Perdew correlation functional P86 [8]. This functional was chosen due to the limited number of empirical parameters used in it and the ability to take into account various types of electron correlation in the calculations of metal complexes.

The calculations were performed using the GAUSSIAN 16 software package [9] in a valence-split basis of Gaussian contracted atomic orbitals 6-31*g*(*d*) with the addition of polarisation *d*-orbitals for a correct description of the symmetry of metal electron levels. The abbreviation 6-31 means that the filled electron layers are described by one set of six contracted primitive Gaussians, and the valence layers are described by two sets of three contracted and one uncontracted primitive Gaussians. In addition, during the calculation of the total electron energies of the crystal and its fragments, an energy correction was taken into account due to the incompleteness of the finite basis set of atomic orbitals. The temperature used in the calculations was set at 295 K.

## 3. Experimental procedure

The elastic moduli of a metal can be calculated based on the displacement (sagging deflection) of the centre of the plate (substrate) onto which the metal film is applied [10]. Based on the results of such measurements, the elastic modulus is determined as follows:

$$E = \frac{FL^3}{4ab^3y}, \quad (7)$$

where $F$ is the external force under which the plate is bent; plate dimensions: $L$ (length), $b$ (thickness), $a$ (width); $y$ is the sagging deflection.

Experimental studies were carried out on nickel and copper plates with a rectangular cross-section of dimensions $L$ = 119 mm, $b$ = 0.5 mm, $a$ = 12 mm. Young's modulus was determined by the bending deformation of the plates before and after applying electrolytic films of pure nickel and copper, as well as composite nickel-copper coatings containing particles of carbon nanomaterial.

Metal coatings with a thickness of 20-25 μm were deposited from aqueous electrolyte solutions with the following compositions, in g/l: nickel plating electrolyte: $NiSO_4\ 7H_2O$ – 300, $H_3BO_3$ – 30, $Na_2SO_4\ 10H_2O$ – 50, pH – 5; copper plating electrolyte: $CuSO_4\ 5H_2O$ – 250; $H_2SO_4$ – 75, pH –0-1. Ultradisperse diamond nanoparticles (UDD) were used as the carbon nanomaterial, with a concentration of 2 g/l in the aqueous electrolyte solution. Deposition was carried out at a temperature of 293–298 K using rectangular current pulses with a frequency ($f$) of 50 Hz, a pulse duty cycle ($Q$) of 50, pulse duration ($t_u$) of 0.4 ms, and average current density ($j_{av}$) of 100 A/m$^2$ for nickel plating and 200 A/m$^2$ for copper plating. A comparison was made with composite coatings obtained using direct current.

To study the fine structure of the films, we used an X-ray DRON-2.0 diffractometer with scintillation registration of X-rays. The phase composition of the films was determined using monochromatic Cu- and Co-*K*α radiations. Annealed nickel and copper were used as standards. The dislocation density was estimated based on the true physical broadening of the diffraction line. The crystal lattice period was determined based on the visible maximum of the diffraction line, taking into account its width and correction for the measurement geometry.

Table 1. Young's moduli of nickel, copper and CEC based on them

| Metal | | $a$, nm | ρ, $cm^{-2}$ | $W_{total}$, $10^{-19}$J | [hkl] | $V_{hkl}$, $10^{-30}$ $m^3$ | $\Delta V_{hkl}$, $10^{-30}$ $m^3$ | $W_{hkl}$, $10^{-19}$ J | $\Delta W_{hkl}$, $10^{-19}$ J | $E_{hkl}$, GPa | $E_{exp}$, GPa |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Ni | single crystal | 0.3524 | --- | 21116.56 | [100] | 43.810 | 0.0438 | 21116.494 | 0.081 | 185 | --- |
| | | | | | [110] | 43.807 | 0.0439 | 21116.483 | 0.0926 | 211 | |
| | DC | 0.3521 | 1.,3×$10^{10}$ | 21115.17 | [100] | 43.660 | 0.0436 | 21115.097 | 0.0720 | 166 | 172 |
| | | | | | [110] | 43.658 | 0.0440 | 21115.086 | 0.0832 | 189 | |
| Ni+UDD | DC | 0.3521 | 7.9×$10^{10}$ | 21115.22 | [100] | 43.660 | 0.0436 | 21115.293 | 0.0730 | 168 | 180 |
| | | | | | [110] | 43.658 | 0.0440 | 21115.303 | 0.0834 | 190 | |
| Ni+UDD | PC (*f*=50 Hz, Q=50) | 0.3514 | 8.5×$10^{10}$ | 21115.82 | [100] | 43.400 | 0.0430 | 21115.898 | 0.0780 | 181 | 194 |
| | | | | | [110] | 43.309 | 0.0443 | 21115.911 | 0.0913 | 206 | |
| Cu | single crystal | 0.3615 | --- | 22967.15 | [100] | 47.290 | 0.0472 | 22967.102 | 0.0450 | 95 | --- |
| | | | | | [110] | 47.289 | 0.0474 | 22967.089 | 0.0574 | 121 | |
| | DC | 0.3613 | 0.8×$10^{10}$ | 22966.86 | [100] | 47.210 | 0.0471 | 22966.819 | 0.0380 | 80 | 82 |
| | | | | | [110] | 47.210 | 0.0467 | 22966.807 | 0.0490 | 105 | |
| Cu+UDD | DC | 0.3613 | 3.5×$10^{10}$ | 22966.74 | [100] | 47.210 | 0.0471 | 22966.701 | 0.0390 | 84 | 86 |
| | | | | | [110] | 47.210 | 0.0467 | 22966.689 | 0.0510 | 110 | |
| Cu+UDD | PC (*f*=50 Hz, Q=50) | 0.3610 | 7.0×$10^{10}$ | 22966.11 | [100] | 47.110 | 0.0471 | 22966.067 | 0.0430 | 92 | 107 |
| | | | | | [110] | 47.113 | 0.0472 | 22966.053 | 0.0566 | 120 | |

## 4. Results and discussion

To reduce the discrepancies between theoretical calculations using formula (1) and the values of Young's modulus of polycrystalline materials determined by the bending method, mainly due to the presence of defects, it was necessary to model the crystal structure as close as possible to the real one. For this purpose, studies of the fine structure of electrodeposited films were carried out, after which the films were tested by the bending method.

Table 1 shows the Young's modulus values for copper and nickel with a FCC lattice, calculated using formula (1) for single crystals and real crystals ($E_{hkl}$), and compares them with experimental data ($E_{exp}$). Table 1 shows that the results of calculating the Young's modulus using a quantum mechanical approach are in good agreement with experimental values and literature data [11-13]. In addition, the dependence of the influence of structural defects on the Young's modulus value can be traced.

X-ray structural analysis showed that during deposition using direct current, an equilibrium structure with few defects is formed in the films (Table 1). In the pulsed deposition mode ($f$ =50 Hz, Q=50), the crystal lattice period decreases and the dislocation density increases. Composite electrolytic coatings obtained under the same conditions have the highest dislocation density, which is due to a decrease in crystallization stress, leading to a more non-equilibrium crystallization process [14, 15].

It is known that with a decrease in the lattice parameter, i.e., with the convergence of atoms, interatomic bonds become stronger, and the Young's modulus should increase, which is observed for an ideal, defect-free crystal. Real materials contain defects, in particular dislocations. Studies show that an increase in dislocation density (ρ) first leads to a decrease and then to an increase in Young's modulus, which correlates well with the hypothetical Oding diagram [16].

The Young's modulus values calculated using formula (1) are in good agreement with the results of other researchers. For example, in [17], for polycrystalline nickel $E$=210 GPa and for a single crystal in the [100] direction $E_{100}$=140 GPa; for polycrystalline copper $E$=125 GPa and for a single crystal in the [100] direction $E_{100}$=68.4 GPa. In [18], the following values are given for polycrystalline materials: for nickel $E$=196 GPa and for copper $E$=131 GPa.

The distance between atoms varies depending on the crystallographic directions. This determines the anisotropy of the mechanical and physical properties of the crystal. Therefore, samples cut from a single crystal in different directions have different Young's modulus values. In a face-centred lattice, there are three main planes with the densest packing of atoms, which are designated (100), (110), (111). These planes have the minimum surface energy. FCC metals have the highest Young's modulus in the [111] direction, while the lowest one – in the [100] direction. Real materials consist of a multitude of randomly oriented single crystals, which leads to the isotropy of their properties.

## 5. Conclusions

The proposed quantum-mechanical approach within the framework of the density functional theory allows calculating the elastic modulus of single- and polycrystalline materials in various crystallographic directions. The obtained calculated values of the elastic modulus of Ni and Cu polycrystals, as well as the CEC based on them in the [100] and [110] directions are in good agreement with the results of experimental measurements obtained by the bending method. The obtained values of Young's modulus can be used to find the shear modulus and to determine the energy required for the introduction of an adsorbed atom into the metal matrix.

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