EFFECT OF A DIELECTRIC COATING OF THE METAL SURFACE ON THE ELECTRON WORK FUNCTION

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In the frame of the Kohn–Sham self-consistent method, we have calculated the electron work function, contact potential difference, and surface stress of the elastically deformed faces of Al, Au, Cu, and Zn crystals with a dielectric coating. The dielectric coating decreases the work function and increases the contact potential difference. The calculations showed the opposite behaviors of the work function of electrons and the contact potential difference under deformation. It is shown that the measurements of the contact potential difference of a deformed face by the Kelvin method correspond to a variation of the one-electron effective potential on the plane of the virtual image behind the surface, rather than to a change of the electron work function. The calculated quantities are in agreement with the results of both experiments for polycrystals and first-principles calculations.

1. Introduction

Till now, a certain bulk of the results of experimental and theoretical studies of the field and thermoelectron emissions, as well as the dependences of the work function and the contact potential difference on a deformation and a dielectric coating of metal specimens [1–9].

The measurements based on the Kelvin method have shown the dependence of the Volta potential φ on a deformation of the surfaces of metal specimens. By this dependence, one can estimate the parameters of a stressed state of a metal: the value of residual mechanical stresses, the structure of dislocations, and corrosion resistance. The chemical activity related to a value of the surface energy or the tension is also sensitive to the surface deformation [6,7].

In connection with the perspective development of nanotechnologies, for example, the formation of nanoclusters on metal films with a dielectric coating, the creation of molecular transistors on this basis [10,11], and the diagnostics of such structures, the problem of the interrelation of surface tension, work function, and measured contact potential difference is urgent.

In the recent works [3–7], the direct measurements of φ in the processes of uniaxial, two-axis, or bending deformation of plane Al, Cu, steel, Zn, and Ni specimens were performed (the references on earlier experiments are given in [10]). The work function was calculated (as it is accepted in the Kelvin method) by the formula

$$\varphi = \frac{W - W_{\perp}}{-e}, \tag{1}$$

where e is the elementary positive charge, and $W_{\perp}$ is the work function of electrons from a probe [6,7].

Despite the fact that similar measurements have been carried on for a long time, there exists no unambiguous opinion about the interrelation of the contact potential difference and the work function up to now (see, e.g., [12]). The answers to some questions, including the work function anisotropy which was numerically studied within the method of density functional, are given in [13–15].

The dependence of the work function on a dielectric coating was calculated by the direct variational method in the earlier works (see references in [16]) and by the Kohn–Sham method for a Na nanowire in the model of “ordinary” jellium [17].

The purpose of the present work is the calculation of energy characteristics of the elastically deformed metal surface coated by a dielectric and the interpretation of the relevant recent experiments [3–7], in which the dependence of the contact potential difference of the stressed surface of Al, Cu, Au, and Zn in air or in various gaseous media was measured.

2. Model of the Surface

In the frame of the method of density functional, the total energy of a *bounded* metal crystal is a functional of the inhomogeneous electron concentration $n(\mathbf{r})$, $n(\mathbf{r}) \to \bar{n}$ in the metal bulk, $\bar{n} = 3/4\pi r_s^3$, $r_0 = Z^{1/3} r_s$, r_0 and r_s are, respectively, the mean distances between ions and electrons in the bulk of the unstressed metal, and Z is the valency.

In the pseudopotential approximation (the model of stable jellium), the total energy can be written in the form of a sum

$$E[n(\mathbf{r})] = T_\mathrm{s} + E_\mathrm{xc} + E_\mathrm{H} + E_\mathrm{ps} + E_\mathrm{M}, \tag{2}$$

where T_s is the kinetic energy of noninteracting electrons, E_xc is the exchange-correlation energy, E_H is the (electrostatic) Hartree energy, E_ps is the pseudopotential correction, and E_M is the Madelung energy. The sum of three first terms in (2) corresponds to the energy of an "ordinary" (unstable) jellium.

The model of a deformed surface and the scheme of a deformation (Fig. 1) are comprehensively presented in [15]. Here, we consider only the necessary details which arise mainly due to the presence of a dielectric coating.

As a rule, a semiinfinite metal is described with the use of the elecron profile $n(\mathbf{r})$ and the effective potential $v_\mathrm{eff}(\mathbf{r})$ which vary only in the direction normal to the face of the surface under study. The commonly accepted approach admits the use of periodic boundary conditions in the x- and y-directions. Hence, we assume the presence of crystallographic planes normal only to the z-direction. In this case, the system of Hartree–Fock–Kohn–Sham equations looks as

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + v_\mathrm{eff}[z,n]\right]\psi_k(z) = \frac{\hbar^2 k^2}{2m}\psi_k(z), \tag{3}$$

$$n(z) = \frac{1}{\pi^2}\int\limits_0^{\bar{k}_\mathrm{F}} dk\,\left(\bar{k}_\mathrm{F}^2 - k^2\right)|\psi_k(z)|^2\,. \tag{4}$$

The effective potential

$$v_\mathrm{eff}[z,n(z)] = e\phi(z) + v_\mathrm{xc}(z) + \langle\delta v\rangle_\mathrm{face}\,\theta(-z) \tag{5}$$

is written in the approximation of local density. The electrostatic potential

$$\phi(z) = \phi(\infty) - 4\pi e\int\limits_z^\infty dz'\int\limits_{z'}^\infty dz''\frac{[n(z'') - \rho(z'')]}{\epsilon(z'')} \tag{6}$$

is obtained by the integration of the Poisson equation with the boundary condition $\phi(z) \to 0$ at great distances from the metal. For example, the function $\epsilon(z)$ for the semiinfinite metal – semiinfinite dielectric contact is equal to 1 inside the metal and ε behind its surface, ε is the dielectric constant. The distribution of the ionic charge is modeled by the jump-like function $\rho(z) = \bar{n}\theta(-z)$. The term $\langle\delta v\rangle_\mathrm{face}$ (5) independent of the coordinates allows one to distinguish different faces of a crystal [13, 15, 18].

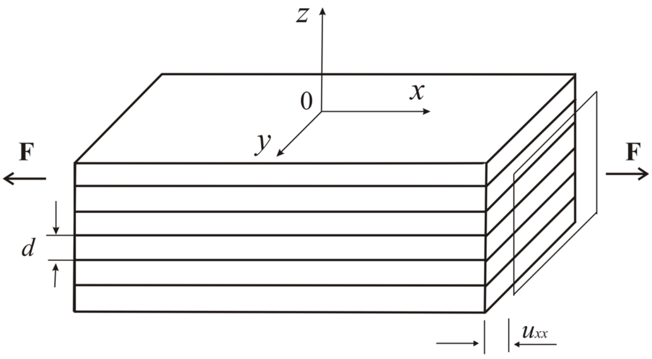

Fig. 1. Qualitative scheme of the elastic uniaxial tension of a specimen under the action of a force **F**; d is the distance between crystallographic planes

The model in use describes the structure of a metal "on the average", like in the model of "ordinary" jellium. Therefore, we describe a dielectric on the surface only with the use of the dielectric constant ε, as it is accepted within the approximation of continuous medium.

The thickness of a dielectric на the surface of a semiinfinite metal is foreseen to be less than the free path of an electron (tens of Å) injected into this dielectric. As will be shown in what follows, the electron profile drops sharply (approximately at a distance of 10–15a_0) in the dielectric. For comparison, we recall that the diameter of molecule O_2 equals $6a_0$. Therefore, the calculations are executed under the assumption that the dielectric is semiinfinite. This simplifies the calculation of the electrostatic potential by the iteration procedure.

The wave number vary in the interval (0, $\bar{k}_\mathrm{F}$). In order to find a self-consistent solution of the system of equations (3), (4), and (6) for $n(z)$ and $\phi(z)$, we used the iteration procedure.

3. Self-Consistency Procedure

In the model of stable jellium, a metal i sdescribed only by the parameters Z, r_s, and d (d is the distance between crystallographic planes which is the argument of the function $\langle\delta v\rangle_\mathrm{face}$ in (5)). By setting the relative deformation u_{xx}, we will calculate a change of the cell volume with the use of the Poisson's ratio. This leads to a change of r_s, $\bar{n}$ as a consequence, and also d (values of the parameters are taken from [15,21]).

By solving Eq. (6), the initial approximation was taken in the form of a one-parameter trial function [19]

$$n^{(i-1)}(z) = \bar{n}f(z),$$

$$f(z)=\begin{cases}1-\frac{1}{2}\exp(z/L), & z<0,\\ \frac{1}{2}\exp(-z/L), & z>0,\end{cases} \tag{7}$$

whose optimality is determined by the condition $\gamma(L,[\bar{n}])\to\min$ for the surface energy at a given value of $\bar{n}$ (L is the variation parameter). For such a function, the electrostatic potential is obtained by the substitution of (7) in the Poisson equation with the following integration:

$$\phi^{(i-1)}(z)=-4\pi\bar{n}L^2 f(z), \tag{8}$$

where i is the iteration number.

After the determination of the initial approximation of the electrostatic potential by formula (8), we calculated the effective potential (5). Then, by solving the differential equation (3), we determined the wave functions and substituted them after the normalization in Eq. (4). In such a way, we determine the distribution of the electron concentration $n^{(i)}(z)$. Then we again calculated the electrostatic potential $\phi^{(i)}(z)$. Such a procedure was repeated until the electrostatic potential $\phi^{(i)}(+\infty)$ at the i-th iteration step differs from $\phi^{(i-1)}(+\infty)$ at the $i-1$-th step less than by 10^{-8} eV.

In order to determine the electrostatic potential $\phi^{(i)}(z)$, it is necessary to solve the one-dimensional Poisson equation at each i-th step of the iteration procedure. To this end, the one-dimensional Poisson equation is rewritten in the form

$$\frac{d^2\phi(z)}{dz^2}-q^2\phi(z)=-\frac{4\pi e}{\epsilon(z)}[n(z)-\bar{n}\theta(-z)]-q^2\phi(z). \tag{9}$$

We introduced the term $q^2\phi$ as a small perturbation. This is the standard procedure of the numerical solution of such differential equations.

Equation (9) was solved by the Lagrange method. The solution has the form

$$\phi_1^{(i)}(z)=\int\limits_{-\infty}^{0}dz'\,U_1e^{-q|z-z'|}+$$

$$+C_1e^{qz}+C_2e^{-qz},\ z\le 0, \tag{10}$$

$$\phi_2^{(i)}(z)=\int\limits_{0}^{\infty}dz'\,U_2e^{-q|z-z'|}+$$

$$+C_3e^{qz}+C_4e^{-qz},\quad z\ge 0, \tag{11}$$

where

$$U_1=\frac{2\pi e}{q}[n^{(i-1)}(z')-\bar{n}]+\frac{q}{2}\phi^{(i-1)}(z'), \tag{12}$$

$$U_2=\frac{2\pi e}{q}\,\frac{n^{(i-1)}(z')}{\varepsilon}+\frac{q}{2}\phi^{(i-1)}(z'). \tag{13}$$

The constants $C_{1,2,3,4}$ remain unknown. The boundary conditions

$$\frac{d\phi_1^{(i)}}{dz}\Big|_{z=0}=\varepsilon\frac{d\phi_2^{(i)}}{dz}\Big|_{z=0},\quad \phi_1^{(i)}\Big|_{z=0}=\phi_2^{(i)}\Big|_{z=0},$$

$$\frac{d\phi_1^{(i)}}{dz}\Big|_{z=-\infty}=0,\quad \frac{d\phi_2^{(i)}}{dz}\Big|_{z=+\infty}=0 \tag{14}$$

give a system of four equations (14), whose solution has the form

$$C_1=\frac{2\varepsilon}{\varepsilon+1}\int\limits_{0}^{b}dz'\,U_2e^{-qz'}+\int\limits_{a}^{0}dz'\,U_1e^{qz'}, \tag{15}$$

$$C_2=e^{2qa}\int\limits_{a}^{0}dz'\,U_1e^{-qz'},\ C_3=e^{-2qb}\int\limits_{0}^{b}dz'\,U_2e^{qz'}, \tag{16}$$

$$C_4=\frac{2}{\varepsilon+1}\int\limits_{a}^{0}dz'\,U_1e^{qz'}+\frac{\varepsilon-1}{\varepsilon+1}\int\limits_{0}^{b}dz'\,U_2e^{-qz'}, \tag{17}$$

where a and b are the lower and upper limits of the integration with respect to z, respectively. The result can be simplified, because $C_2\to 0$ as $a\to-\infty$ and $C_3\to 0$ as $b\to\infty$. It is convenient to take $q=\bar{k}_{\rm F}$.

At $\varepsilon=1$, formulas (10) and (11) can be rewritten in the form

$$\phi^{(i)}(z)=\int\limits_{-\infty}^{\infty}dz'\Big\{e^{-\bar{k}_{\rm F}|z-z'|}\frac{2\pi e}{\bar{k}_{\rm F}}[n^{(i-1)}(z')-\rho(z')]+$$

$$+\frac{\bar{k}_{\rm F}}{2}\phi^{(i-1)}(z')\Big\}. \tag{18}$$

[The self-consistent scheme in [20], which was used in the calculation of the binding energy of a positron at the vacancy of a metal, is also reduced to formula (18).]

Assuming the value of the electrostatic potential in vacuum far beyond the scope of a metal coated by a dielectric to be zero, $\phi(+\infty)$ =0, we can calculate the work function of electrons in the metal–dielectric–vacuum system in the z-direction,

$$W\equiv-\mu=-\bar{v}_{\rm eff}-\bar{\varepsilon}_{\rm F}, \tag{19}$$

and a component of the surface tension

$$\tau_{xx}=\gamma+d\gamma/du_{xx}, \tag{20}$$

where μ is the chemical potential of electrons, γ is the specific surface energy of a face, and u_{xx} is the relative deformation.

The bulk value of the effective potential $\bar{v}_{\mathrm{eff}} < 0$ gives the full height of a barrier on the metal face–vacuum interface, and $\bar{\varepsilon}_{\mathrm{F}} = \hbar^2 \bar{k}_{\mathrm{F}}^2/2m > 0$ is the Fermi energy reckoned from the planar bottom of the conduction band.

4. Results of Calculations and Their Discussion

As a test, we firstly calculated the characteristics of pure and unstrained surfaces of polycrystalline metals Cs, Rb, K, Na, Ba, Li, Sr, Ca, Pb, Mg, Al, and Cu. Our results coincide with the data in work [18], where the characteristics of these metals were calculated as well.

The quantity $\langle \delta v \rangle_{\mathrm{face}}$ included in the effective potential allows us to construct the profiles of electron concentrations for planes with different indices which were used in calculations of the observable quantities. The greatest surface energy and the least work function correspond to the face $\langle 110 \rangle$ of an fcc lattice.

In the Table, we compare the calculated and experimental values of the specific surface energy γ and the work function W for polycrystals of Al, Au, Cu, and Zn. Both collections of the data are in a good agreement. The *ab initio* calculations performed in [9] give $\gamma_{\mathrm{face}} = 1.114;\ 1.343;\ 1.372$ J/m^2 and $W = 5.65; 5.56; 5.42$ eV for Au(111), (100), and (110), respectively (see also Table 1 in [9]).

Calculations of the characteristics for deformations $-0.04 \leq u_{xx} \leq +0.04$ display the almost linear dependences of surface characteristics on deformations. A positive/negative deformation u_{xx} means the decrease/increase of the mean concentration of electrons $\bar{n}$ and the tension/compression of the upper face of a specimen, i.e. the decrease/increase of the package density of atoms and the interplane distance in the direction normal to the z axis.

Calculated/experimental values of the specific surface energy γ and the work function W for polycrystals of Al, Au, Cu, and Zn

Metal	Z	r_{s} (a_0)	γ (J/m^2)	W (eV)
Al	3	2.07	0.926/1.160	4.30/4.25^a(4.28^b)
Au	3	2.09	0.912/1.134	4.28/4.30^a(5.10^b)
Cu	2	2.11	0.893/1.351	4.26/4.40^a(4.65^b)
Zn	2	2.31	0.739/0.772	4.10/3.62^a

Note: The experimental values of the specific surface energy γ are taken from [21–23], and the experimental values of the work function W: a – [24], b – [25].

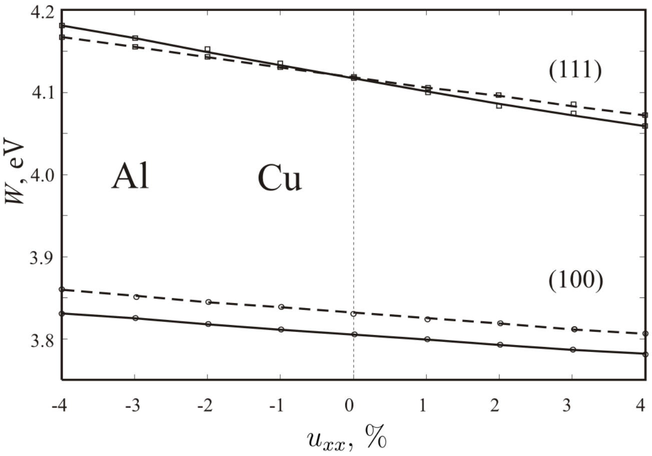

Fig. 2. Dependence of the work function on the uniaxial deformation: Al – solid lines, Cu – dashed lines

In the process of deformation, we observe the almost linear growth of the surface energy. This means that the quantity $d\gamma/du_{xx}$ is positive both for $u_{xx} > 0$ and $u_{xx} < 0$. Relation (20) gives a value of the surface stress τ_{xx} which is somewhat greater than $\gamma(u_{xx} = 0)$. For $u_{xx} > 0$, the value of τ_{xx} is also somewhat greater than that for $u_{xx} < 0$.

The value of surface tension $\tau = 1.376$ J/m^2 calculated for Al(111) by formula (20) well agrees with the results of *ab initio* calculations (1.441 [26]; 1.249 J/m^2 [27]) and is significantly less than values obtained in [28,29]. For example, $d\gamma/du_{xx}$ for trivalent gold in [28] is much greater than γ. The calculations performed in [9] gave significantly greater values $\tau = 3.317;\ 2.723;\ 2.020$ J/m^2 for Au(111), (100) and (110), respectively, (see also Table 1 in [9]) which are not strongly different from results in [30–32]. We note that, in the calculation of τ_{zz} and τ_{yy} for a specimen stretched or compressed along the x axis, it is necessary to use $d\gamma/du_{xx}$ taken for $u_{xx} < 0$ or $u_{xx} > 0$, respectively. The reason lies in that the tension along the x direction leads to the compression of the specimen in the orthogonal directions.

According to Fig. 2, the work function decreases linearly with increase in u_{xx}. The relative variation if this quantity is approximately 1% for planes (111) and (100) and 0.1% for (110). It turned out that the dominant reason for the decrease in W with increase in u_{xx} is the change of $\langle \delta v \rangle_{\mathrm{face}}$. On the whole at the tension, ΔW is determined by negative changes in the values of the electrostatic $e\bar{\phi}$ and exchange-correlation $\bar{v}_{\mathrm{xc}}$ components of the effective potential $\bar{v}_{\mathrm{eff}} = e\bar{\phi} + \bar{v}_{\mathrm{xc}} + \langle \delta v \rangle_{\mathrm{face}}$ and by positive change of the quantity $\langle \delta v \rangle_{\mathrm{face}}$.

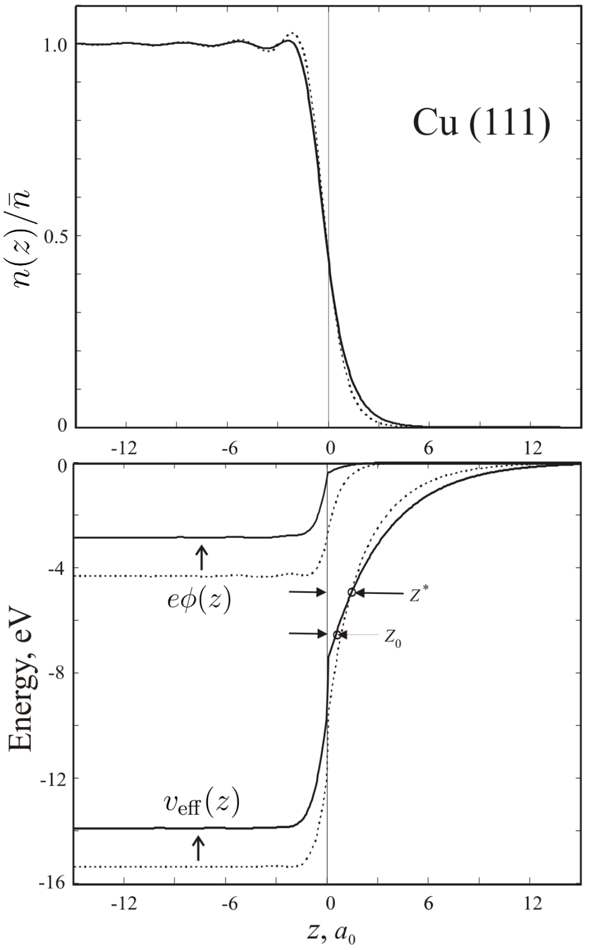

Fig. 3. Results of self-consistent calculations of the electron profile $n(z)$ and the one-electron effective $v_{\rm eff}(z)$ and electrostatic $\phi(z)$ potentials for face Cu(111) coated by the dielectric: $\varepsilon = 10$ (solid lines) and $\varepsilon = 1$ (dotted line). $z = z^*$ shows the position of the plane, on which a change of the effective potential as a result of the deposition of a coating is zero. The position of the "image plane" $z = z_0 < z^*$ is shown conditionally

The dominant role is played by the change of $\langle \delta v \rangle_{\rm face}$, whereas a change of the Fermi energy is insignificant.

We now carry on the comparison with experimental data from [4,5]. It follows from Fig. 5 in [4] that the change of the work function for the polycrystalline surface of Cu at the uniaxial tension/compression is $-0.04/+0.02$ eV on the boundary of the elastic and plastic regions. Our result $-0.03/+0.03$ eV agrees by sign and magnitude with these values. A good agreement is also obtained for Al [5].

The results of calculations [9] in the interval $u_{xx} = \{-0.04, +0.04\}$ demonstrated the change of the chemical potential of electrons $\Delta\mu = 0.08$, 0.05, and 0.15 eV for Au (100), (110), and (111), respectively, which is consistent by sign with our results but exceeds them approximately twice. We recall that μ and W have different signs [see (20)].

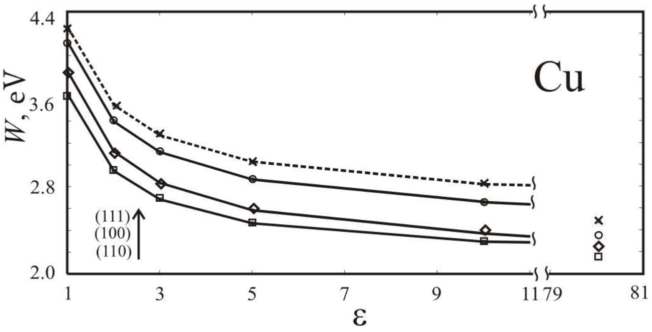

Fig. 4. Dependences of the work function of electrons on the dielectric constant ε of the coating calculated for some faces of monocrystals (solid lines) and polycrystalline surfaces (dashed line)

In view of the multimolecular thicknesses of dielectric coatings or oxides on a metal surface and a rapid fall of the electron distribution outside of a metal, we can *formally* neglect the effect of a thickness of this coating, whose minimum thickness must be much greater than that of a monoatomic (molecular) layer of a dielectric. Such an assumption allows us not to consider the boundary conditions on the dielectric-vacuum interface on solving the Poisson equation. Therefore, for convenience of calculations, we set that the thickness of a dielectric is infinite, and the coating has the same elastic properties, as a metal. The last circumstance is related to that a metal and a dielectric have, in fact, different elastic properties. Therefore, the metal-dielectric interface can be really warped, which cannot be taken into account in our model.

The effect of a dielectric coating on the surface is reduced to the "elongation" of the electron distribution tail and the effective potential beyond the surface of a metal (Fig. 3). On the boundary of the metal and the coating, there occurs the jump of the derivative of the electrostatic potential $d\phi(z)/dz$ which is absent if the dielectric constant of the coating equals unity. The calculations were performed for $\varepsilon = 1, \dots, 5, 10$, and 80. In this case like in [17] for a nanowire of Na placed in a dielectric, an increase in ε leads to a decrease in the depth of the potential well ($|\bar{v}_{\rm eff}|$ decreases), in which the electrons in the metal are positioned. For this reason, the electron work function decreases (Fig. 4). The curve $W(\varepsilon)$ tends to the "saturation". The calculations are especially difficult for the (110) plane of a fcc lattice and plane (0001) of a hexagonal lattice due to the least value of interplane distance d, on which the stabilization potential $\langle \delta v \rangle_{\text{face}}$ depends.

The deformation gradient of the work function in the presence of a dielectric coating is independent, in fact, of ε. With increase in ε, the effect of a coating is reduced to a shift downward on the energy scale of all curves $W(u_{xx})$ in Fig. 2 in the presence of a deformation.

The results obtained are in qualitative agreement with experiments, in which one observed a decrease of the work function due to the presence of an inert dielectric: Kr on the W(112) surface [33] (see also Fig. 6.1 in [2]) and paraffin and polyethylene on Al or Zn [6]. However, if the reaction of oxidation is running on the surface (Zn in humid air), the measurement of the Volta potential (Fig. 1 in [6]) demonstrate an increase of the work function according to formula (1) within the Kelvin method. The replacement of humid air by dry one (see the experiment in [6]) leads to the opposite change of the Volta potential. We may assume that, in addition to the oxidation of the surface, the water vapor brings a negative charge. This charge firstly leaks partially in a metal and then, after the formation of an oxide, remains in the thin water layer on the surface. This charge is removed then by dry air together with water. The presence of a noncompensated charge is apparently revealed in the measurements through a more negative Volta potential and an increase of the work function.

By definition (1), a change of the Volta potential due to a perturbation of the surface (the charging, a deformation, or the coating with a dielectric) is

$$-e\Delta\varphi = \Delta W. \tag{21}$$

It was concluded in works [13,14] that the Kelvin method allows one to register changes of the surface potential due to a deformation; therefore, the interpretation of the results of measurements of the Volta potential must be based on the analysis of a change of the effective potential $\bar{v}_{\text{eff}}$ near the surface under the action of a deformation rather than on a variation of the work function. The Kelvin method fixes the potential beyond the geometric surface of a body on the image plane, relative to which the electrostatic image is constructed, i.e. on the plane $z = z_0$ (see Fig. 3). As distinct from the work function W (to which $\langle \delta v \rangle_{\text{face}}$ directly contributes, because its value is nonzero only in the interior of a specimen), the effective potential at the point $z = z_0$ "feels" a deformation with the help of the procedure of self-consistency of the solution of the Kohn–Sham equations. Therefore, we use, instead of (21),

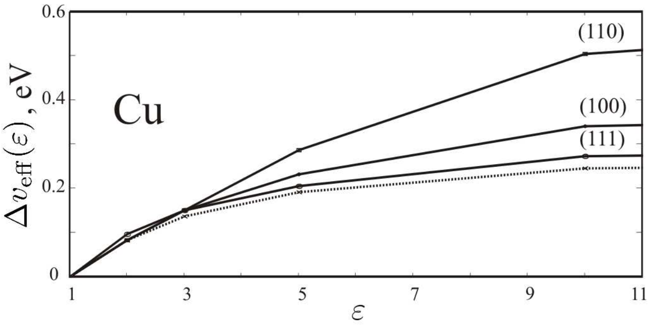

Fig. 5. Variation of the effective potential $\Delta v_{\text{eff}}(\varepsilon) \equiv v_{\text{eff}}(z_0, \varepsilon) - v_{\text{eff}}(z_0, \varepsilon = 1)$ on the virtual image plane as a function a dielectric constant for three faces (solid lines) and the surface of a polycrystal (dotted line)

$$\Delta\varphi = \Delta v_{\text{eff}}(z_0, \varepsilon, u_{xx})/e. \tag{22}$$

For different faces of different metals, $z_0 \simeq 1\, a_0$ [10]. The calculations of $v_{\text{eff}}(z)$ for Cu (111) executed at $\varepsilon = 1$ and $u_{xx} = 0, +4$ % gave the relation $\Delta v_{\text{eff}}(z = z_0, u_{xx}) \equiv v_{\text{eff}}(z_0, +4\%) - v_{\text{eff}}(z_0, 0) = \alpha \Delta v_{\text{eff}}(z = -\infty, u_{xx})$, where $\alpha \simeq -1.4$. As a result of the fact that a change of the Fermi energy is slight [see definition (19)], we have

$$\Delta v_{\text{eff}}(z = -\infty, u_{xx}) \simeq \Delta W.$$

For Al (111), we get $\alpha \simeq -3$. This means that, in the process of deformation, values of the effective one-electron potential in the bulk (a position of the conduction band bottom) and beyond the surface are shifted to the opposite sides on the energy scale. Thus, $\Delta\varphi$ (Fig. 5) and ΔW differ both by sign and absolute magnitude.

As follows from Fig. 3, there exists such a plane $z = z^*$, on which the difference $v_{\text{eff}}(z^*, \varepsilon) - v_{\text{eff}}(z^*, \varepsilon = 1)$ becomes zero. Because z^* and z_0 are close to each other, and the real surface is far from the ideal one, the measurements of the Volta potential can give the values of $\Delta\varphi$ opposite by sign, which is indeed observed in experiments.

For the quantitative comparison with the data of experiments, the obtained values of work function for different planes should be averaged, since a polycrystalline specimen is the collection of arbitrarily oriented monocrystallites. In this case, the qualitative answer will not be changed, because the deformation gradients have the same sign for different crystallographic faces of metals.

The inhomogeneous distribution of the Volta potential observed in [6,7] on the surfaces of stressed planar and bent *finite* specimens shows, as if, the nonequipotentiality of the metal surface. According to classical electrodynamics, the equipotentiality of the surface is probably ensured on the much greater distance than the gap between a probe and the surface.

5. Conclusion

The surface tension, electron work function, and contact difference of the potentials of elastically strained faces of crystals of Al, Cu, Au, and Zn are calculated in the model of stable jellium. A dielectric coating causes a decrease of the work function and an increase of the contact difference of potentials. The calculations demonstrated a decrease/increase of the work function and a increase/decrease of the contact potential difference on the homogeneous tension/compression of the surface of a metal crystal. The results correspond to the direct observation of a shift of the contact potential: values of the effective potential beyond faces of a specimen shift to the side of negative/positive values if a tensile/compressive force acts. The result does not depend on a metal and a crystallographic direction: the change of the work function has the same tendency as φ, but not the inverse one, as it was shown by calculations based on the direct variational method and simple trial functions [10].

The results obtained can be used in the diagnostics of metal films in electronics for the presence of a dielectric coating on the surface or dislocations in the metal bulk. By determining the surface characteristics, one can control the processes of formation of thin adsorbed polymeric films on metals and the deposition of oxides.

As a very important point, we mention the problem of the protection of metals against corrosion. The determination of the surface energy or the surface tension allows one to estimate the chemical activity of a surface and, in particular, its corrosion resistance.

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ВПЛИВ ДІЕЛЕКТРИЧНОГО ПОКРИТТЯ МЕТАЛЕВОЇ ПОВЕРХНІ НА РОБОТУ ВИХОДУ ЕЛЕКТРОНІВ

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Резюме

Роботу виходу електронів, контактну різницю потенціалів та поверхневу напругу пружно деформованих граней кристалів Al, Au, Cu та Zn з діелектричним покриттям розраховано в рамках самоузгодженого методу Кона–Шема. Діелектричне покриття зменшує роботу виходу і збільшує контактну різницю потенціалів. Розрахунки демонструють протилежні деформаційні залежності роботи виходу електронів і контактної різниці потенціалів. Показано, що вимірювання методом Кельвіна контактної різниці потенціалів деформованої грані відповідають не зміні роботи виходу електронів, а зміні значення одноелектронного ефективного потенціалу на площині уявного зображення за поверхнею. Розраховані величини узгоджуються з результатами експериментів для полікристалів і розрахунків із перших принципів.