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Simple theory of elastically deformed metals: Surface energy, stress, and work function

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The effect of uniaxial strain on surface properties of simple metals is considered within the stabilized jellium model. The modified equations for the stabilization energy of the deformed Wigner-Seitz cells are derived as a function of the bulk electron density and the given deformation. The model requires as input the density parameter r_s, the Poisson ratio, and Young's modulus of the metal. The results for surface energy, surface stress, and work function of simple metals calculated within the self-consistent Kohn-Sham method are also presented and discussed. A consistent explanation of the independent experiments on stress-induced contact potential difference at metal surfaces is given.

I. INTRODUCTION

The early experimental investigations of the force acting on electron inside a metallic tube in the earth's gravitational field[1] posed a question about the influence of metal deformation upon the electronic work function. The direct measurements, using the Kelvin method, showed a decreasing/increasing of the contact potential difference (CPD) of the tensed/compressed metal samples.[2–5] Similarly, the experiment with a high speed spinning metal rotor, which was nonuniformly deformed over the length, demonstrated that CPD changes between the areas of the surface subjected to different deformation[6] (see also discussion of earlier experiments by Harrison[7]). The influence of deformation upon electronic emission from a thin metallic film has been also investigated.[8] Recently, a similar effect on the CPD was observed at the surface of sample with a nonuniform distribution of residual mechanical stress.[9] At first sight, these results seem to be surprising because they mean the respective increase/decrease of the work function with decreasing/increasing electron density that is caused by a uniaxial tension/compression of metalic sample. Therefore, all these experiments stimulate two important questions which should be answered by the microscopic theory: (i) Does the change of the CPD correspond to a change in the work function? (ii) Which sign will have the deformation gradients of surface energy and work function for a metal that is subject to the tensile (or compressive) strain along some direction?

From the general statement of the theory of elasticity follows that the change in the total energy of a solid is proportional to the square of relative deformation. Therefore, the energy must increase so for compression as for tension. On the other hand, experimentally it was found that in the range of elastic deformation, a uniaxial strain of metallic sample leads to a linear change in the CPD.[3–5] This implies that classical theory of elasticity may be not completely adequate in determination of the elastic characteristics of metal surfaces.

The second question is of importance by the determination of surface tension or surface stress.[10] Gohstein[11] have demonstrated that the measurements of the derivative of surface tension of a solid with respect to the electrical variables showed a small difference between the surface stress and surface energy. On the other hand, different calculations,[12–14] including the ones based on the first principles,[14–16] point to the appreciable difference between these two quantities. A rough estimation of the difference between surface energy γ and surface stress g which can be done using the cohesive energy and the vacancy formation energy[17] shows that g is approximately equal to or less than γ.

In this work we address the questions raised above by investigating theoretically the surface energy, surface stress, and work function of elastically deformed metal. A uniaxial strain applied to the surface introduces anisotropy to the metal by changing the density (or separation) of atomic planes, electron gas concentration, and contributes to an extra surface dipole barrier. A rigorous study of this problem from first principles is tedious and requires heavy numerical computations.[14–16] On the other hand, the calculations based on the isotropic models of metal, i.e., on the jellium model,[10,18] which ignores the discrete nature of ions, or the stabilized jellium model,[12,13,19] in which interparticle interactions are averaged over the volume of spherical Wigner-Seitz cells, do not allow proper accounting for the effects of inhomogeneous strain. In the present work we develop a modification of a stabilized jellium model,[13,19,20] in order to describe the deformed metal.[12,13,21] In this modification the metal energy is expressed as a function of the density parameter r_s and of the given deformation. Section II presents equations for a stabilized jellium model accounting for elastic deformation. In Sec. III, the modified stabilized jellium model is applied to calculate, by the Kohn-Sham method, the effect of a uniaxial strain on the electronic surface characteristics of single crystals of aluminum and lithium.

II. MODEL OF DEFORMED METAL

The dependence of the CPD on the uniaxial deformation was measured for polycrystalline samples.[4,5] Let us consider

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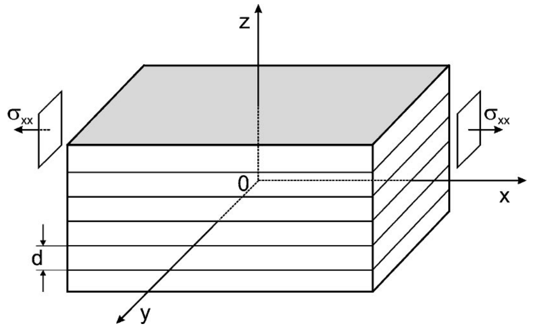

FIG. 1. Qualitative sketch of the crystal deformed (expanded) in the x direction. d is the interplanar distance. The calculations are performed for the upper, shaded side of the crystal.

a hypothetical crystal in the shape of a rectangular parallelepiped (Fig. 1). In the undeformed state all of its faces are equivalent. We assume that deformation is a measured quantity and a metallic crystal is to be considered as assembled from a number of simple crystallites. Thus, qualitatively, the problem can be reduced to the consideration of tension or compression applied to a single crystal.

Let us first express the average electron density in a metal $\overline{n}$ as a function of deformation. For this purpose, consider an undeformed cubic cell of the side length a_0 and volume

$$\Omega_0=a_0^3=\frac{4}{3}\pi r_0^3, \tag{1}$$

where $r_0=Z^{1/3}r_s$ is the radius of the spherical Wigner-Seitz cell, Z is the valence, $r_s=(3/4\pi n_0)^{1/3}$, and n_0 is the average electron density in the bulk of undeformed crystal. For a uniaxially deformed cell, elongated or compressed along the x axis, one can write

$$\Omega=a_x a_y^2=\frac{4}{3}\pi a b^2, \tag{2}$$

where a_x and $a_y=a_z$ are the sides of the elementary parallelogram, and a and b are the half-axes of the equivalent prolate or oblate spheroid of revolution relative to the x axis. Denoted by u_{xx} the uniaxial strain we have

$$a_x=a_0(1+u_{xx}) \quad \text{and} \quad a_z=a_0(1+u_{zz})=a_0(1-\nu u_{xx}), \tag{3}$$

where $\Omega/\Omega_0-1=u_{xx}+u_{yy}+u_{zz}$, and ν is the polycrystalline Poisson coefficient (ratio) that is relating[22] the transversal compression to the elongation in the direction of applied deformation, i.e., $u_{yy}=u_{zz}=-\nu u_{xx}$. From Eqs. (1)–(3) follows

$$a=r_0(1+u_{xx}) \quad \text{and} \quad b=r_0(1-\nu u_{xx}). \tag{4}$$

Similarly, the spacing between the lattice planes perpendicular to the y or z directions is

$$d_u=d_0(1-\nu u_{xx}), \tag{5}$$

where d_0 is the interplanar spacing in an undeformed crystal. Consequently, following Eqs. (1)–(4), the average electron density in the deformed metal is given by

$$\overline{n}=n_0\Omega_0/\Omega=n_0[1-(1-2\nu)u_{xx}]+O(u_{xx}^2), \tag{6}$$

and the corresponding density parameter is

$$r_{su}=r_s[1+(1-2\nu)u_{xx}]^{1/3}. \tag{7}$$

Having defined the basic parameters for the strained system let us consider its energy in order to obtain the condition for stability. Proceeding similarly as for the derivation of equations for the original stabilized jellium model,[19] we consider a metal assembled from the Wigner-Seitz cells. The average energy per valence electron in the bulk is

$$\varepsilon_{SJ}=\varepsilon_J(\overline{n})+\varepsilon_M+\overline{w}_R, \tag{8}$$

where the first term gives the jellium energy

$$\varepsilon_J(\overline{n})=\frac{3}{10}k_F^2(\overline{n})-\frac{3}{4\pi}k_F(\overline{n})+\varepsilon_{cor}(\overline{n}), \tag{9}$$

consisting of the average kinetic and exchange-correlation energy per electron with k_F being Fermi momentum, $k_F^3=3\pi^2\overline{n}$. (We employ atomic units throughout.) The remaining two terms in Eq. (8) represent the Madelung energy and the average of the repulsive part of the Ashcroft model potential. A small, band structure energy term[19] is neglected in Eq. (8).

As usual for isotropic medium, by transformation of the ordinary jellium into a stabilized one, the Coulomb interactions were averaged over the Wigner-Seitz cell. The uniaxial strain applied to the crystal deforms the spherical Wigner-Seitz cells into ellipsoidal ones. This has an influence on the Madelung energy ε_M which now should be averaged over the volume of the deformed cell. It can be expressed in the form similar to the gravitational energy of the uniform spheroid[23] to give

$$\begin{aligned}\varepsilon_M(\overline{n})&=\frac{1}{Z}\int_{\text{spheroid}}d^3r\,\overline{n}\left(-\frac{Z}{r}\right)+\frac{1}{2Z}\int_{\text{spheroid}}d^3r\,\overline{n}V(r)\\&=-\frac{9Z}{10a}\sum_{k=0}^{\infty}C_k\frac{p^{2k}}{2k+1},\end{aligned} \tag{10}$$

where $V(r)$ is the electrostatic potential inside a uniformly charged spheroid, $C_k=\{1,u_{xx}>0;(-1)^k,u_{xx}<0\}$, and $p=\sqrt{|1-b^2/a^2|}$ defines the spheroid's eccentricity. The series appearing in Eq. (10) can be expressed by analytical functions.[24] This expression has a correct limit: $\varepsilon_M(\overline{n})\rightarrow-0.9Z/r_0$ for $u_{xx}\rightarrow 0$.

We assume that the shape of ionic cores is not influenced by the deformation and they remain spherical, thus the averaging of the Ascroft empty-core pseudopotential gives

$$\overline{w}_R=2\pi\overline{n}r_c^2. \tag{11}$$

For the averaged difference $\delta v(\mathbf{r})$ between the ion pseudopotential and the potential of the uniform positive background, holds the same relation[19] as for the unstrained crystal, i.e.,

$$\langle\delta v\rangle_{WS}=\tilde{\varepsilon}+\varepsilon_M+\overline{w}_R, \tag{12}$$

where the electrostatic self-energy of the uniform negative background inside a spheroid is

$$\tilde{\varepsilon} = -\frac{2}{3}\varepsilon_M . \tag{13}$$

The pseudopotential core radius r_c can be fixed from the condition of mechanical equilibrium depending on the mechanical stress induced in the volume of the cell. In order to determine the core radius let us note that for the strained metal the intrinsic pressure in the bulk of metallic sample

$$P = -\frac{dE}{d\Omega} = \bar{n}^2 \frac{d\varepsilon_{SJ}}{d\bar{n}} \tag{14}$$

is compensated by the pressure exerted by the external forces

$$P = -(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) = -Yu_{xx}(1-2\nu), \tag{15}$$

where σ_{ii} are the components $(i=x,y,z)$ of the tensor of mechanical stress and Y is the Young's modulus[22] defined as $\sigma_{ii} = Yu_{ii}$. It should be noted that for the ideal metal $\nu = 1/2$ and $P=0$. It means that the applied external force does not change the volume but the shape of a cell or sample.

Consequently, the average energy per electron in the bulk of a strained metal can be written as

$$\varepsilon = \varepsilon_J(\bar{n}) + \varepsilon_M + \bar{w}_R + P/\bar{n}, \tag{16}$$

where ε, standing on the left side of Eq. (16), is considered to be the energy which minimizes at the equilibrium density for the strained metal, treating P as a given constant fixed by Eq. (15). In the linear approximation, Madelung energy (10) is well approximated by $\varepsilon_M(\bar{n}) \rightarrow -0.9Z/r_{0u}$. Inserting the latter and for the particular terms in Eq. (16) the explicit expressions from Eqs. (9) and (11)–(13), from the minimum energy condition $d\varepsilon/d\bar{n} = 0$ we have

$$r_c = \left\{ -\frac{2}{15}\left(\frac{9\pi}{4}\right)^{2/3} r_s + \frac{1}{6\pi}\left(\frac{9\pi}{4}\right)^{1/3} r_s^2 + \frac{1}{5}Z^{2/3}r_s^2 + \frac{2}{9}r_s^4 \frac{d\varepsilon_{\mathrm{cor}}}{dr_s} + \frac{8}{9}\pi r_s^6 P \right\}^{1/2}_{r_s = r_{su}}, \tag{17}$$

where r_{su} is the equilibrium density parameter of the strained metal. Here, we assume that the volume of the spheroid is equal to the volume of the equivalent sphere of radius $r_{0u} = Z^{1/3}r_{su}$. As can be seen, the pseudopotential core radius now depends upon the strain u_{xx}. One would not expect this from pseudopotential theory, where the pseudopotential should transfer unchanged from one environment to another, but it is a consequence of forcing a first-order pseudopotential model to do the work of a higher-order model. Thus Eq. (17) assures transferability only for the equally strained systems (in the regime of linear strains).

Making use of the equality[19]

$$\langle \delta v \rangle_{WS} = \bar{n}\frac{d}{d\bar{n}}(\varepsilon_M + \bar{w}_R), \tag{18}$$

we get at the equilibrium density corresponding to a strained metal:

$$\langle \delta v \rangle_{WS} = -\bar{n}\frac{d}{d\bar{n}}[\varepsilon_J(\bar{n}) + P/\bar{n}]. \tag{19}$$

Consequently, Eqs. (16), (17), and (19) allow us to construct the total energy of a finite strained crystal with a surface, as a functional of the electron density, and of the form originally derived by Perdew *et al.*[19] but with r_c and $\langle \delta v \rangle_{WS}$ determined from Eqs. (17) and (19), respectively.

Subsequently, in order to calculate the face-dependent surface properties, similarly as Perdew *et al.*[19,13] we can replace the stabilization potential (19) by the following form:

$$\langle \delta v \rangle_{\mathrm{face}} = \langle \delta v \rangle_{WS} - \left(\frac{\varepsilon_M}{3} + \frac{\pi \bar{n}}{6} d_u^2 \right), \tag{20}$$

where the second term on the right side of Eq. (20) represents the dipole barrier due to atomic corrugations at the surface.[19,20]

The total energy of a finite rectangular crystal confined by the walls of area A_x and $A_y = A_z$, may be written as the sum of the bulk E^b and surface E^s energy where

$$E^s = \gamma_y 4A_y + \gamma_x 2A_x . \tag{21}$$

Here, $\gamma_y = \gamma_z$ and γ_x are surface energies, per unit area, of the lateral and base sides, respectively. In the undeformed state $\gamma_x = \gamma_y = \gamma_z \equiv \gamma$, and surface energy (21) changes by

$$dE^s = 4A_y\left(\gamma\delta_{\alpha\beta} + \frac{d\gamma}{du_{\alpha\beta}} \right) du_{\alpha\beta} + 2A_x\left(\gamma\delta_{\alpha\beta} + \frac{d\gamma}{du_{\alpha\beta}} \right) du_{\alpha\beta}, \tag{22}$$

where α and β denote directions in the plane of lateral and base sides and $\delta_{\alpha\beta}$ is the Kronecker delta. The expressions in the braces represent the components of surface stress. Following the model presented in this work we calculate only

$$g_{xx} = \gamma + \frac{d\gamma}{du_{xx}}. \tag{23}$$

By definition,[13] putting the electrostatic potential in the vacuum equal zero, for a certain face of semi-infinite crystal, the electron work function can be written as

$$W_{\mathrm{face}} = -\bar{\phi} - \frac{d}{d\bar{n}}[\bar{n}\varepsilon_J(\bar{n})] - \langle \delta v \rangle_{\mathrm{face}}, \tag{24}$$

where, $\bar{\phi} < 0$ denotes the electrostatic potential in the metal bulk. Alternatively, work function can be calculated from the displaced-profile change-in-self-consistent field expression.[25] For a discussion of our results presented in the subsequent section, it is useful to rewrite Eq. (24) in the following form:

$$W_{\mathrm{face}} = -\bar{v}_{\mathrm{eff}} - \varepsilon_F, \tag{25}$$

where the effective potential[20,26] in the bulk, $\bar{v}_{\mathrm{eff}} = \bar{\phi} + \bar{v}_{\mathrm{xc}} + \langle \delta v \rangle_{\mathrm{face}}$, gives the total barrier height at the metal-vacuum interface, $\bar{v}_{\mathrm{xc}}$ is the exchange-correlation potential in the bulk $[\bar{v}_{\mathrm{xc}} \equiv v_{\mathrm{xc}}(-\infty)]$, and $\varepsilon_F = \frac{1}{2}k_F^2$ is the Fermi energy.

TABLE I. Calculated surface energies γ, work function W_{face}, strain derivative $d\gamma/du_{xx}$, and surface stress $g=g_{xx}$, for elastically deformed Al ($r_s=2.06$) and Li ($r_s=3.25$) samples. Positive and negative deformations $u_{xx}=\pm 0.03$ are labeled with $(+)$ and $(-)$. ΔW_{face} is the difference of the work function for a strained and unstrained surface. The values of Young's modulus are: 70 GPa (Al) and 11.47 GPa (Li) (Ref. 27).

Metal	Face	γ (erg/cm^2)	W_{face} (eV)	u_{xx}	$\frac{d\gamma}{du_{xx}}$ (erg/cm^2)	g (erg/cm^2)	ΔW_{face} (eV)
Al	(111)	946	4.096	$+$	460	1406	-0.032
				$-$	400	1346	0.033
	(100)	1097	3.780	$+$	833	1930	-0.025
				$-$	810	1907	0.016
Li	(110)	311	3.286	$+$	20	330	-0.011
				$-$	13	324	0.011
	(100)	345	3.037	$+$	37	382	-0.005
				$-$	37	382	0.005

III. APPLICATION AND DISCUSSION

To verify the theory presented in Sec. II, the Kohn-Sham equations were solved for the two most densely packed surfaces of Al and Li represented by the stabilized jellium model.[26] In the language of our model, we consider two regular single crystals of Al (and Li) which in undeformed state have all of their sides equivalent. Owing to the crystal deformation the four of the side-faces remain equivalent to one another, but not to the two base faces (Fig. 1). The $\langle \delta v \rangle_{\text{face}}$ term included into the effective potential allows the generation of the face-dependent density profiles[20,26] which were used to calculate the surface characteristics: work function, surface energy, and surface stress. All calculations were carried out for the upper side of the sample (see Fig. 1) assuming the polycrystalline value of the Poisson coefficient, $\nu=0.36$,[27] for elastic properties of both Al and Li.

Within the applied range of deformation, $-0.03 \leqslant u_{xx} \leqslant 0.03$, the changes in surface quantities remain linear. The positive/negative strain u_{xx} means expansion/compression of the side of a sample, i.e., the decrease/increase of the atomic packing density at this side, and the decrease/increase of the mean electron concentration $\bar{n}$ and interplanar spacing in the direction perpendicular to the considered crystal side. For a better understanding of the physical effects we have also performed calculations for the special case of the ''ideal'' metal for which $\nu=1/2$. In this case the deformation does not change $\bar{n}$, however, the second term (corrugation dipole barrier) in the face-dependent potential (20) will be changed.

The results of calculations are summarized in Table I. As is seen the surface energy increases linearly with the applied positive deformation u_{xx} and decreases with the negative one. It means that $d\gamma/du_{xx}$ is positive both for $u_{xx}>0$ and for $u_{xx}<0$. Accordingly, Eq. (23) gives values of the component of surface stress g_{xx} larger than surface energy. For $u_{xx}>0$ surface stress is somewhat larger than for $u_{xx}<0$. The changes are more noticeable for Al than for Li. It seems that the classical definition of surface stress[28,29] works better for the ideal metal. This is connected with the fact, that subjected to deformation, ideal metal changes only its surface area—the electron concentration in its bulk remains unchanged. The calculations performed for Al(111) surface yield the values of the strain derivative $d\gamma/du_{xx}=247$ and 213 erg/cm^2, for $u_{xx}>0$ and $u_{xx}<0$, respectively. These values are much smaller than the ones reported in Table I. In this case $(\nu=1/2)$ we can also evaluate the other components of surface stress $g_{zz}=g_{yy}=\gamma+d\gamma/du_{yy}$. Substituting $du_{zz}=du_{yy}=-\nu du_{xx}$ we get $g_{zz}=g_{yy}=\gamma-2d\gamma/du_{xx}<\gamma$. Let us make two observations at this point. First, the latter result agrees with the results derived on the basis of the elasticity theory[30] where the g/γ ratio was expressed in terms of the Poisson coefficient, ν, to give $(3\nu-1)/(1-\nu)$. For $\nu=1/2$, this formula gives $g/\gamma=1$, and $g<\gamma$, for $\nu<1/2$. Second, in order to calculate g_{zz} and g_{yy} for a sample expanded along the x axis we should exploit the value of $d\gamma/du_{xx}$ for $u_{xx}<0$, whereas for a compressed sample, the corresponding value for $u_{xx}>0$. This is because the tension applied along the x direction causes a sample to be compressed along the orthogonal (y and z) axes, cf. Eq. (3). For Al(111) the calculated surface stress (Table I) is in a very good agreement with the values resulting from the available ab initio calculations: 1249 erg/cm^2[16] and 1441 erg/cm^2[14]. It gives also improvement over the results obtained for ordinary jellium[12,16] and our previous direct application of the stabilized jellium model.[12]

For the considered strains the work function decreases linearly with u_{xx}, but the relative change is less than 1% (see Table I). The similar behavior is observed for $\nu=1/2$. It is seen that the dominating component, which leads to a decrease of W with u_{xx}, is a change in the $\langle \delta v \rangle_{\text{face}}$ term. Thus, the change of work function under the influence of deformation is determined by the competition of negative change both in the exchange-correlation v_{xc} and electrostatic ϕ components of the effective potential v_{eff} and the positive change in the face-dependent component $\langle \delta v \rangle_{\text{face}}$. A dominant role is played by the change of $\langle \delta v \rangle_{\text{face}}$ term while the change in the Fermi energy is quite unnoticeable. An overall decrease/increase in the work function W is determined by a positive/negative shift of the electrostatic potential in the metal interior.

The calculated change of the work function with strain seems to contradict the experimental results[2–6] where it was found that work function increases/decreases with elongation/compression of the sample. This conclusion was based on the analysis of the measured CPD.[2–7,9,21] For the

TABLE II. Calculated change in the effective potential $\Delta v_{\text{eff}}(z=z_0)$ at the surface of elastically deformed and neutral sample of Al ($r_s=2.06$) and Li ($r_s=3.25$). Positive and negative deformations $u_{xx}=\pm 0.03$ are labeled with (+) and (−).

Metal	Face	u_{xx}	$\Delta v_{\text{eff}}(z_0)$ (eV)
Al	(111)	+	−0.103
		−	0.106
	(100)	+	−0.064
		−	0.069
Li	(110)	+	−0.014
		−	0.015
	(100)	+	+0.015
		−	−0.012

conventional method of measurement of the work function changes upon strain,[3–5] this means that $W(u_{xx})=W(0)-\Delta V(u_{xx})>W(0)$, i.e., the work function increases for a tensed sample. Here ΔV denotes the CPD. In the following we argue that this contradiction is spurious. The point is that the measurement by Kelvin method fixes the change of surface potential. So, the explanation of experimental observations can be given based not upon the change in the work function but by analyzing the change in the effective potential v_{eff} upon deformation. The Kelvin method gives the value of the potential difference at the surface of a sample which one can define as the position of the image plane $z=z_0$.[26] Note that in distinction to the work function, to which $\langle \delta v\rangle_{\text{face}}$ term contributes directly [Eq. (24)], at the image-plane position (which is located outside the geometric surface) $\langle \delta v\rangle_{\text{face}}$ equals zero and there the effective potential feels the change in $\langle \delta v\rangle_{\text{face}}$ only by means of the self-consistent procedure. The calculations performed for Al(111) and Li(110) demonstrate that the ratio of the effective potential difference Δv_{eff} between strained ($u_{xx}=\pm 0.03$) and strain-free samples, at the surface and in the bulk, is $\Delta v_{\text{eff}}(z=z_0)/\Delta \overline{v}_{\text{eff}}\approx 0.8$. Here, $\Delta \overline{v}_{\text{eff}}$ denotes the respective difference in the metal bulk.

The results for $\Delta v_{\text{eff}}(z_0;u_{xx})$ are shown in Table II. The potential difference outside the sample becomes more negative as deformation increases, with the exception of Li(100). The calculated changes in the effective potential have the same sign as the measured CPD for Al. For a polycrystalline Al sample subject to deformation $u_{xx}=0.03$, the CPD amounts to -0.025 ± 0.002 V.[4,5] Since a polycrystalline sample can be considered as assembled from arbitrarily oriented single crystals, the values obtained by us should be averaged in order to compare them with experiment. As is seen both experiment and calculations give a negative change of the surface potential, $\Delta V=\Delta v_{\text{eff}}(z=z_0)<0$. Thus, taken as a whole our results agree with the independent experiments both for expanded[3–6] and compressed[1,2] metallic samples. The results for $\Delta v_{\text{eff}}(u_{xx})$ correspond to direct observation of stress-induced shift in the measured contact potential: The effective potential outside the open faces of a sample is more negative/positive when tensile/compressive force is applied. However, unlike the effective potential at the surface, due to the different effect of the $\langle \delta v\rangle_{\text{face}}$ term, the value of the potential in the metal bulk is more positive/negative for an expanded/compressed sample. So, for the Al sample the work function change vs strain shows an opposite trend compared to that of contact potential. It differs also from that predicted by non-self-consistent calculations.[4,21] Accordingly, the results of Table I demonstrate that work function decreases with u_{xx}. In other words, our results show that the measurements by Kelvin method do not give a change in the work function but a change in the surface potential upon strain.

In summary, the stabilized jellium model has been extended to encompass the effects of elastic strain on surface properties of simple metals. By imposing uniaxial strain to metal surface and limiting ourselves to linear terms in deformation, we have obtained a realistic description of strain dependence of surface quantities: surface energy, surface stress, and work function. We have presented a consistent explanation of experiments on stress-induced contact potential difference at metal surfaces. The elasticity effects considered in this work may play an important role in the explanation of recently observed force and conductance fluctuations in the tensed metallic nanowires.[31,32]

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