

QUANTUM SIZE EFFECTS IN FINITE METALLIC NANOWIRES

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Abstract

The size dependence of the electronic density of states, Fermi energy, and the ionization potential of a finite metallic nanowires is systematically investigated in a free-electron, finite-potential well model for Au and Al. Anisotropy of work function is discussed. A nanowire is modelled by a uniform conductor of a finite length and square cross-section. Simple relation between the Fermi energy and the depth of a square potential well is employed which yields a correct monotonic size-dependence of the ionization potential relative to its bulk value. It is shown that the ionization potential, as a function of the wire width, oscillates around the values provided by this average dependence. The oscillations in the energetic and force properties result from the size quantization of the energy levels. We obtained the force fluctuations in accordance with the experimentally found values. The consequences of the present investigation of the correct amount of force and conductance fluctuation in elongation of point contacts are discussed.

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1. INTRODUCTION

Physical properties of clusters, thin films, quantum dots and other low-dimensional systems attract currently a lot interest [1]. The application of such atomic-size systems in microelectronics and nanotechnology make the question of their electronic structure of critical technological importance. Also the mechanical and electrical properties of the microscopic contacts between metallic bodies are currently a subject of an intensive experimental [2,3] and theoretical [4-7] studies. For example, simultaneous measurement [3] of the force and conductance during elongation of the gold nanowire formed between two electrodes have demonstrated that a stepwise variation of the conductance is accompanied by the fluctuations of the force.

One of the problems in the physics of low-dimensional systems is to determine the size dependence of the surface energy and electron work function. The size dependent work function shows oscillations around the monotonic average dependence. Analytical theory of density of states and the Fermi energy in a free-electron solid of sub-micron dimensions, including their monotonic component and oscillations within infinite potential barrier was developed in [8]. Available numerical results give equivocal answer regarding the size-monotonic component of the Fermi energy. The calculations reported in Ref.9 (Ref.10,11) show that the monotonic component of work function increase/or independent with the width

of the thin films(does not depend on the film width). For infinite nanowires this component slowly increases [12] or decreases [13] with the radius. In this report we discuss the criteria of this dependence, based on the theory for spherical clusters, which is more developed today.

We study the energy and force fluctuations in the finite nanowires as a function of the wire cross section. We consider whiskers of a constant volume and different shape of the surface, neglecting the temperature effects [14].

2. IONIZATION POTENTIAL OF A FINITE SAMPLE

Basic relations. It is important to note that in all experiments we have to do with the *finite* samples. A different reticular electron density at particular faces of single crystal (crystallite) of irregular shape leads to the difference of electrostatic potential for these faces. It seems, as if the work functions along different directions were different for the finite sample. This conclusion is not correct. It is connected with widely-distributed point of view (see [15] and references therein), that the work function "anisotropy" determined by the reticular electron density of the given crystal face. However, the electron work function is defined as the difference between the electron energy level in the vacuum and at the Fermi surface. This difference is independent of space directions and coordinates and is constant for metallic sample. The work function is a scalar quantity. This confirmation follows from the convenient definition for the ionization potential of finite sample (spherical cluster, finite film, whisker etc) is

$$IP = E_{N-1} - E_N, \quad (1)$$

where E_N is the energy of neutral metallic sample that contain N electrons. In the framework of density functional theory the energy E_N is the functional of the electron $n(r)$ and ion $\rho(r)$ densities

$$E_N[n, \rho] = G[n] + E_i[n, \rho] + \frac{e^2}{2\epsilon_0} \int d^3r d^3r' \frac{[n(\vec{r}) - \rho(\vec{r})][n(\vec{r}') - \rho(\vec{r}')]}{|\vec{r} - \vec{r}'|}, \quad (2)$$

where the universal functional G contains the kinetic electron energy and exchange-correlation energy $G[n] = K_e[n] + E_{xc}[n]$, E_i is the energy of ion subsystem. The distribution of the electron density satisfies the normalization condition

$$\int d^3r n(\vec{r}) = N \gg 1.$$

In a large sample the electrons are collectivized therefore the energy of cluster with Z excess electrons can be represented by the functional expansion [16, 17]

$$E_{N+Z}[n(r) + \Delta n(r)] = E_N[n(r)] + \int d^3r \frac{\delta E_N}{\delta n(r)} \Delta n(r) + \frac{1}{2!} \int d^3r d^3r' \frac{\delta^2 E_N}{\delta n(r) \delta n(r')} \Delta n(r) \Delta n(r') + \dots \quad (3)$$

under following normalization condition

$$\int d^3r \Delta n(\vec{r}) = Z, \quad (4)$$

where $\Delta n(r)$ is the distribution of excess electrons. By definition the chemical potential of electron liquid in a neutral finite sample is

$$\mu_N = \delta E_N / \delta n(r). \quad (5)$$

In general, for any sample we have

$$E_{N+Z} = E_N + Z\mu_N + \frac{e^2}{2\varepsilon_0} \int d^3r d^3r' \frac{\Delta n(\vec{r}) \Delta n(\vec{r}')}{|\vec{r} - \vec{r}'|}, \quad (6)$$

where ε_0 is the dielectric constant. Due to intrinsic electrostatic repulsion in an electron liquid the uncompensated charge $-eZ$ is localized at the metal surface. From Eq.(5) for $Z = -1$ follows an expression for IP .

Spherical cluster. Let us represent expression (6) in the analytical form for the spherical cluster. For estimation we choose electronic distribution $\Delta n(r)$ in a convenient form

$$\Delta n(r) = \begin{cases} 0, & 0 < r < R - b \\ n_q, & R - b < r < R \\ 0, & r > R \end{cases}, \quad (7)$$

where b is the thickness of the near-surface layer containing excess electron density n_q . From normalization condition (4) and (7) we obtain the following expression for surface density

$$n_q = \frac{Z}{\Omega(3\xi - 3\xi^2 + \xi^3)}, \quad (8)$$

where $\Omega = 4\pi R^3 / 3$, $\xi = b/R$. Using (7) and (8), straightforward integration in the last term of (6), yields important result

$$\frac{(Ze)^2}{2\varepsilon_0 R} \left(1 + \frac{\xi}{3} + \dots \right).$$

Thus for metallic sphere the principal curvature correction in (6) is independent of the shape of the charge distribution $e\Delta n(r)$. For spherical surface we employ the expansion in power of the inverse radius [18]

$$\mu_N = \mu_0 + \mu_1 / R + \dots \quad (9)$$

For clarity we introduce the definition of the work function of flat surface

$$W_0 = -\mu_0, \quad (10)$$

and one which we will call the “work function of neutral sample”,

$$W_N = -\mu_N. \quad (11)$$

Finally, we have

$$IP = W_N + \frac{e^2}{2C}, \quad (12)$$

where $C = \varepsilon_0 R$ is a capacitance of conductor sphere. It should be mentioned that W_0 and IP are the experimentally measured quantities, but W_N have mainly the methodical sense.

Following the numerous calculations of size dependence of the ionization potential of large spherical rigid [18, 19] and self-compressed [20] clusters, we may assume that one common value of $\mu_1 \approx 0.12$ a.u. can be taken for all simple metals. Since $\mu_1 = \mu_1^{rig} + \delta\mu_1$, where μ_1^{rig} corresponds to a rigid cluster, the value $\delta\mu_1$ accepted by us accounts for the self-compression effects [20]. Then, using (9)-(12) one can write¹

$$W_N = W_0 - \frac{\mu_1}{R} < W_0. \quad (13)$$

In the following, we will assume a universal character of Eq.(12), we will extend it validity for the case of finite nanowires.

Fig.1 shows the curvature dependence $IP(R)$ and $W_N(R)$ for the gold cluster. Let us note that these two quasi-classical dependencies exhibit an opposite size behavior: the $W_N(R)$ increase while $IP(R)$ decreases monotonically with increasing R . This shows a principal difference between the $IP(R)$ and $W_N(R)$: equation (12) can be interpreted as the effect of charging on the curvature dependence of "work function" of neutral finite sample. In other words, it point to a different origin of the size corrections μ_1 / R and $e^2 / 2\varepsilon_0 R$. This

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$$IP = W_0 + \beta \frac{e^2}{C}, \quad (14)$$

where $\beta = \left(\frac{1}{2} - \frac{\mu_1}{e^2}\right) \approx 0.38$. It should be marked that factor β is very close to $\frac{3}{8}$. In spite of the critical discussion [16, 17, 21] is possible this fact confirms the versions of relative redefinition of work function by means of the conception of image potential [22-24] and the uncertainty principle [25].

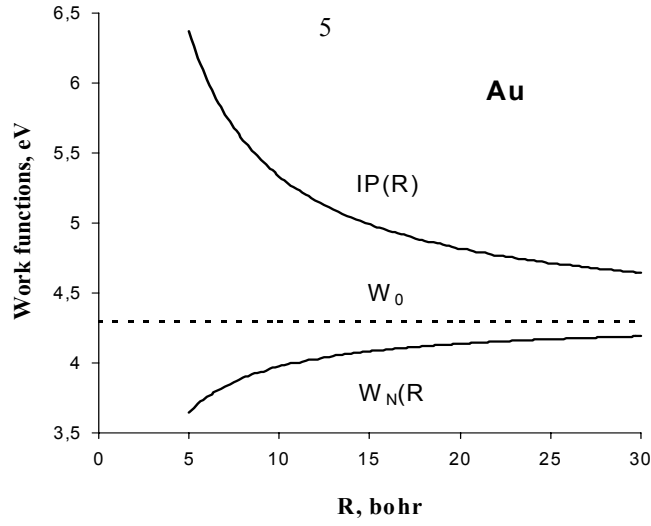


Fig.1. The semi-classical curvature dependences of the “work function of the neutral cluster” $W_N(R)$ and the ionization potential $IP(R)$ for the gold spherical cluster. W_0 is the work function for semi-infinite metal.

difference appears to be useful for the analysis of the energetics of the finite quantum nanowire or the finite quantum film (slab). A wire of infinite length (the same applies to an extended thin slab) has an infinite capacitance, $C \rightarrow \infty$, therefore $IP \rightarrow W_N$. Eq.(13) will be used below as a criterion for the size-dependence of the work function of nanowires-whiskers.

3. ENERGY OSCILLATIONS IN WHISKERS

In this report a finite wire is modelled by a cuboidal enclosure of the length $L_x \equiv L$ and a square cross section of the dimension $L_y = L_z \equiv a \ll L$ (see Fig.2) and the constant volume Ω . In the free electron model the energy spectrum is defined by solution of the one-electron Schrodinger equation with the effective potential $V(r)$. We replace this explicit potential by the square well potential of depth $V_0 < 0$ inside a cluster and zero outside. The electron wave function of the form $\Psi(r) = \psi(x)\psi(y)\psi(z)$ allow to separate the wave equation with respect to x, y and z coordinates. In the y - and z - directions we consider the limit of strong quantization, $k_B T \ll \Delta$, where Δ is the distance between occupied levels, $\max\{n_y, n_z\} \ll \max\{n_x\}$. The length L is assumed to be sufficiently large for spectra of corresponding momentum p_x to form a quasi-continuum. Consequently, the electron energy is $E = p_x^2 / 2m + E_{n_{yz}}$ with $E_{n_{yz}} = E_{n_y} + E_{n_z}$, where n_{yz} is a number of the subband. For an infinitely deep square well this expression reduces to

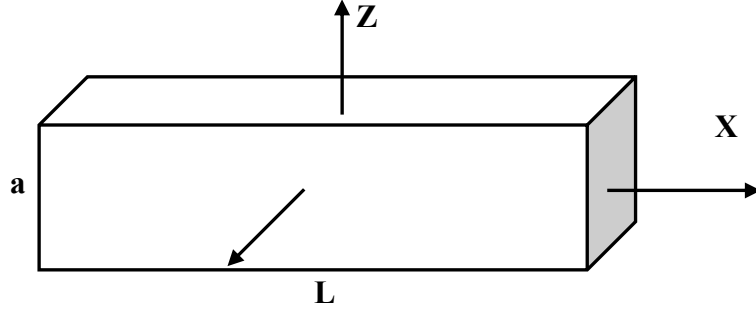


Fig.2. The model nanowire of uniform cross section $a \times a$ and length L .

$$E_{n_{yz}} = \frac{\hbar^2 \pi^2}{2ma^2} n_{yz}^2, \quad n_{yz}^2 = n_y^2 + n_z^2.$$

For $n_y = n_z$, $E_{n_y} = E_{n_z}$. Let us denote

$$-V_0 = \frac{\hbar^2 \chi^2}{2m}, \quad E_{n_z} = \frac{\hbar^2 k_{n_z}^2}{2m}.$$

From the matching conditions for one-electron wave function at the lateral faces of the wire one gets two relations, of identical form, to determine k_{n_z} and k_{n_y} :

$$\tan\left(\frac{1}{2}k_{n_z} a\right) = \pm \left(\chi^2 / k_{n_z}^2 - 1\right)^{\pm 1/2}, \quad (15)$$

where (+) and (-) signs correspond to even and odd stationary states, respectively.

From the practical point of view we employ

$$-V_0 = W_0 + E_F^0, \quad (16)$$

with $E_F^0 = \frac{\hbar^2}{2m}(3\pi^2\bar{n})^{2/3}$ being the Fermi energy of uniform electron system of density $\bar{n} = 3/4\pi r_s^3$, where r_s is the electron density parameter, $r_s = 3.02, 2.07 a_0$ for Au and Al respectively. However, it is well known that the bottom of the cluster potential shows the size oscillations [26,27]. Our aim is to introduce the correct value of V_0 in simple way.

For detail analysis we propose to employ the following three approximations for the bottom of the potential V_0 :

(i) Using (16) and the experimental magnitudes of \bar{n} and $W_0 = 4.3$ and 4.28eV , we get $-V_0 = 9.83$ and 15.19eV for Au and Al respectively. Note that V_0 is independent of the size of a sample.

In the two other variants V_0 was replaced by the following functions of the Fermi energy, E_F , of the considered system,

$$-V(E_F) = W_N(E_F) + E_F, \quad (17)$$

where two functional dependencies for $W_N(E_F)$, based on the Brodie concept [25] of the work function, were used:

(ii) The one proposed to calculate the quantum size effect in the work function of jellium slabs [9],

$$W_N(E_F) = AE_F^{1/4}, \quad (18)$$

and,

(iii) The expression derived [29] by using the length of spontaneous polarization of the electron gas at the Fermi level and the image force action, to give

$$W_N(E_F) = \frac{B}{r_s^{3/2} E_F^{1/2}}. \quad (19)$$

The coefficients A and B are extracted from Eq.(16) for a semi-infinite metal to give: $A = 0.2353, 0.1943$ and $B = 0.3721, 0.3071$ a.u. for Au and Al, respectively. Equation (18) is derived from (19) using relation between r_s and E_F , and give the same results for extended system. However, as will be demonstrate below, for the low-dimensional systems, the different functional dependence of $W_N(E_F)$ on the Fermi energy leads to a different variation of the work function with the wire width. For a finite system, the advantage of one form over the other cannot be unequivocally decided beforehand.

The density of electron states in a wire is defined by the sum,

$$D(E) = \frac{1}{\Omega} 2 \sum_n \delta(E - E_n),$$

over the occupied levels. Replacing the three-dimensional summations over the allowed states in p -space by the ordinary one-dimensional integration over p_x and summation over n_y and n_z , for finite wire, we get

$$D(E) = \frac{L}{\Omega} \sqrt{\frac{2m}{\pi^2 \hbar^2}} \sum_{n_y, n_z}^+ (E - E_{n_{yz}})^{-1/2}. \quad (20)$$

The plus sign in the limit of summation indicates that n_y and n_z run from 1 to the maximum value for which the expression under the square root is positive. Subsequently, the number of electrons in a wire is given by

$$N = \Omega \sum_{n_y, n_z}^+ \int_{E_{n_{yz}}}^{\infty} D(E - E_{n_{yz}}) f(E) dE = \bar{n} \Omega. \quad (21)$$

At low temperatures ($k_B T \rightarrow 0$) the electron distribution function can be represented by a step function $f(E) = \theta(E - E_F)$ and we obtain

$$N = 2L \sqrt{\frac{2m}{\pi^2 \hbar^2}} \sum_{n_y, n_z}^+ (E_F - E_{n_{yz}})^{1/2}. \quad (22)$$

Similarly, the total kinetic energy of electrons in a whisker is given by the integral over energy up to the Fermi energy and summed over all subbands to give

$$K_e = \Omega \sum_{n_y, n_z}^+ \int_{E_{n_{yz}}}^{\infty} D(E - E_{n_{yz}}) f(E) E dE = L \sqrt{\frac{8m}{9\pi^2 \hbar^2}} \sum_{n_y, n_z}^+ (E_F - E_{n_{yz}})^{1/2} (E_F + 2E_{n_{yz}}). \quad (23)$$

The number of electrons N in the whisker is fixed, so by solving simultaneously the set of equations (15) and (22), using (16)-(19), we determine the Fermi energy and then $W_N(E_F)$. In this way the hierarchy of levels in the finite potential well depends self-consistently on the Fermi energy, $E_{n_{xy}} \equiv E_{n_{xy}}(E_F)$.

In order to estimate the $IP(a)$ of a wire we used Eq.(12) and the capacitance of a "needle" in the shape of a prolate spheroid [29]

$$C \cong \varepsilon_0 x_0 (\ln 2\zeta)^{-1}, \quad (24)$$

where x_0 and y_0 are the half-axis of spheroid, and the parameter $\zeta = x_0 / y_0 \gg 1$. A relation between a needle and the wire of square cross section is made by putting $\pi y_0^2 = a^2$ and $x_0 = 3L/4$, subject to a condition of equality of their volumes.

4. FLUCTUATIONS OF THE HOOKE LAW IN WHISKERS

Consider an ideal plastic deformation of the wire that conserves its volume Ω . The tensile force appearing upon elongation of the finite wire is given by

$$F = -dE_N / dL, \quad (25)$$

where E_N is the total energy of the metallic sample containing N electrons.

The total energy of a wire can be decomposed into bulk and surface energies, $E_N = E^b + E^S$, where the bulk energy

$$E^b = K + U,$$

K and U being the total kinetic and potential energy of electron-ion system in the bulk. The surface energy component can be written in the form

$$E^S = \sigma(4aL + 2a^2),$$

where σ is the surface energy per unit area. From the classical virial theorem, for finite electron-ion system, we have

$$U = -2K$$

and consequently, bulk energy of bound system

$$E^b = -K. \quad (26)$$

has a right (negative) sign. For neutral finite wire only electronic contribution, K_e , of the total kinetic energy K depends on the elongation. Therefore one can write

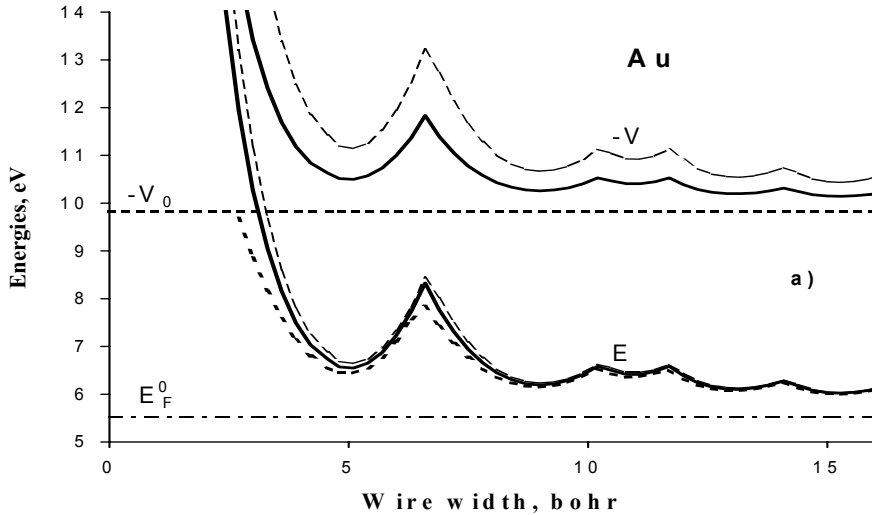
$$F = -\frac{d}{dL}(-K_e + E^S). \quad (27)$$

Thus, Eq.(27) allow to determine variation of the force vs. wire thickness in simple manner. The account for the potential energy of the electron-ion system in Eq.(27) and application of the virial theorem lead to a minus sign in front of the K_e . Note that in Refs.5-7, where a similar simple model of the nanowire has been exploited, an opposite sign appears. The reason for this contradiction is the application of the infinite potential well in [5-7] and neglect of the size dependence of potential energy term in the total energy. Our approach allows to consider a more general case which accounts both for the kinetic and potential energies as functions of the wire width. Eq.(27) is valid for any Coulomb system, when the energy may be separated into bulk and surface components. However, by evaluation of forces from (27) we assume that the derivative of surface energy per unit area $d\sigma/dL = 0$, i.e. the curvature dependence of surface tension is neglected.

It should be mentioned that analogous expression (27) for whisker created in the point contact between two metallic bodies will be written in different form. In this case the wire acquires the surplus charge and two base faces of the wire will be omitted in Eq.(27).

5. RESULTS AND DISCUSSION

Figures 3-5 show the results of calculation of energetic properties of gold and aluminum wires in the (i)-(iii) approximations. We perform calculations for wires of volume $\Omega = 3\text{nm}^3$ in the range of widths $\sqrt{\pi r_s^2} \leq a \leq L/10$. The size dependence of the electronic characteristics, E_F , W_N , and IP of a nanowire was calculated by simultaneous solution of the set of equations (15), (22). As is seen from Fig.3a, the dependence of the Fermi energy on the wire width shows very small differences for the different approximations used. On the other hand, the calculated size dependence $W_N(a)$ plotted in Fig.3b is very sensitive to the applied potential energy form. The work function variations calculated for version (i) and (iii) show reversed character of changes compared to that of model (ii). The correctness of this dependence for a wire is fixed by comparing to the curvature dependence $W_N(R)$ for spherical cluster (see Fig.1). It seems that the best results are supplied by calculations for variant (iii). In this case the bottom of the potential well and the Fermi level show oscillations of the amplitudes less than 1eV. These values are in good accordance with the results of self-consistent Kohn-Sham calculations for spherical clusters and nanowires [12,13,26]. In a more extended calculation it would be interesting to check the evolution of the size dependence of W_N for decreasing dimensionality of the system, i.e., in consecutive series of calculations for a wire (1D), slab (2D) and cluster (3D).



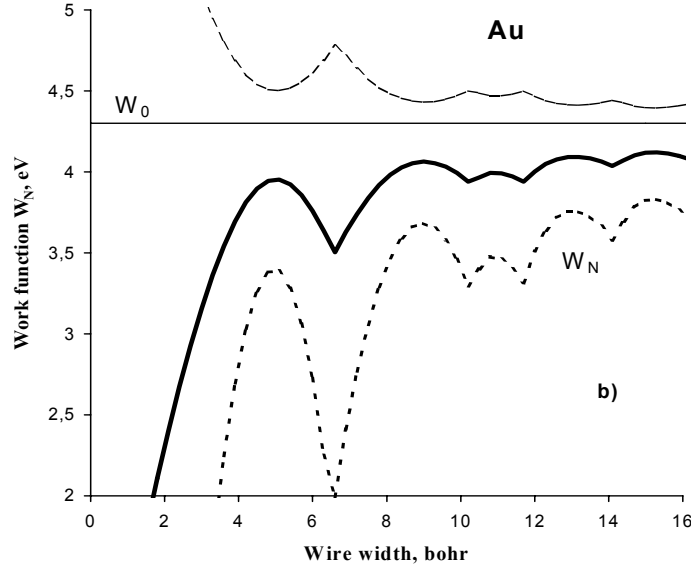


Fig. 3. The results of self-consistent calculations for the depth of potential V in the gold wire, the Fermi energy E_F , and work function $W_N(a)$ performed for three approximations: (i) – short dashed line, $V(E_F) \equiv V_0 = \text{constant}$; (ii) - dashed line; (iii) – solid line. Also the Fermi energy of semi-infinite metal E_F^0 , and work function W_0 are shown.

relative to those of an infinite potential well. It can be explained by the fact that the total kinetic energy of occupied states is sensitive to the actual position of the bottom of the potential well. The peaks in the density of state are more intensive for the additionally degenerate states, $E_{n_y} = E_{n_z}$.

Figure 5 shows a plot of the ionization potential of aluminum whiskers versus the width of the wire, estimated from Eqs.(12) and using the capacity given by (24). The variation of $W_N(a)$ is shown for comparison. As can be seen, there are the ranges of widths, where $IP < W_0$ and $IP > W_0$. The fact that $IP < W_0$ for wires is rather unexpected. Judging from the empirical observation that the work function of the flat metal surface is approximately equal to 0.5-0.8 of the atomic IP , one would expect that the IP of a cluster (independently of the shape of its surface) falls in the range $W_0 < IP(\text{cluster}) < IP(\text{atom})$. This effect has not been observed before and is much greater than the errors connected with the approximate treatment of the capacitance.

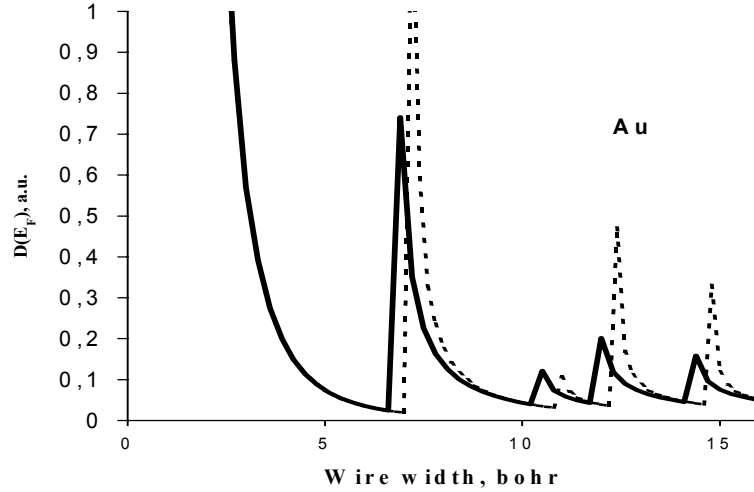


Fig.4. Density of states (DOS) of a gold wire calculated for a finite square potential well (solid curve), and infinite well $V(E_F)$ (dashed curve). The depth of the well V is defined by Eqs.(17) and (19) (approximation (iii)).

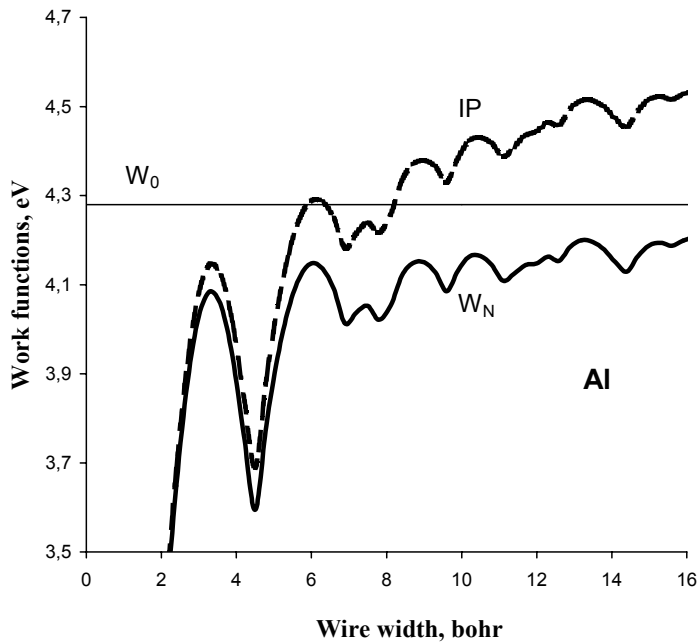


Fig.5. Work function $W_N(a)$ and ionization potential $IP(a)$ of the aluminum whisker, calculated in approximation (iii).

In the limit $a = L$, we deal with a cubic "wire" whose ionization potential must have a value similar to that of a sphere (compare Fig.1). It should be noted that the ionization potential depends only on geometric parameters and is independent of the direction of electron emission.

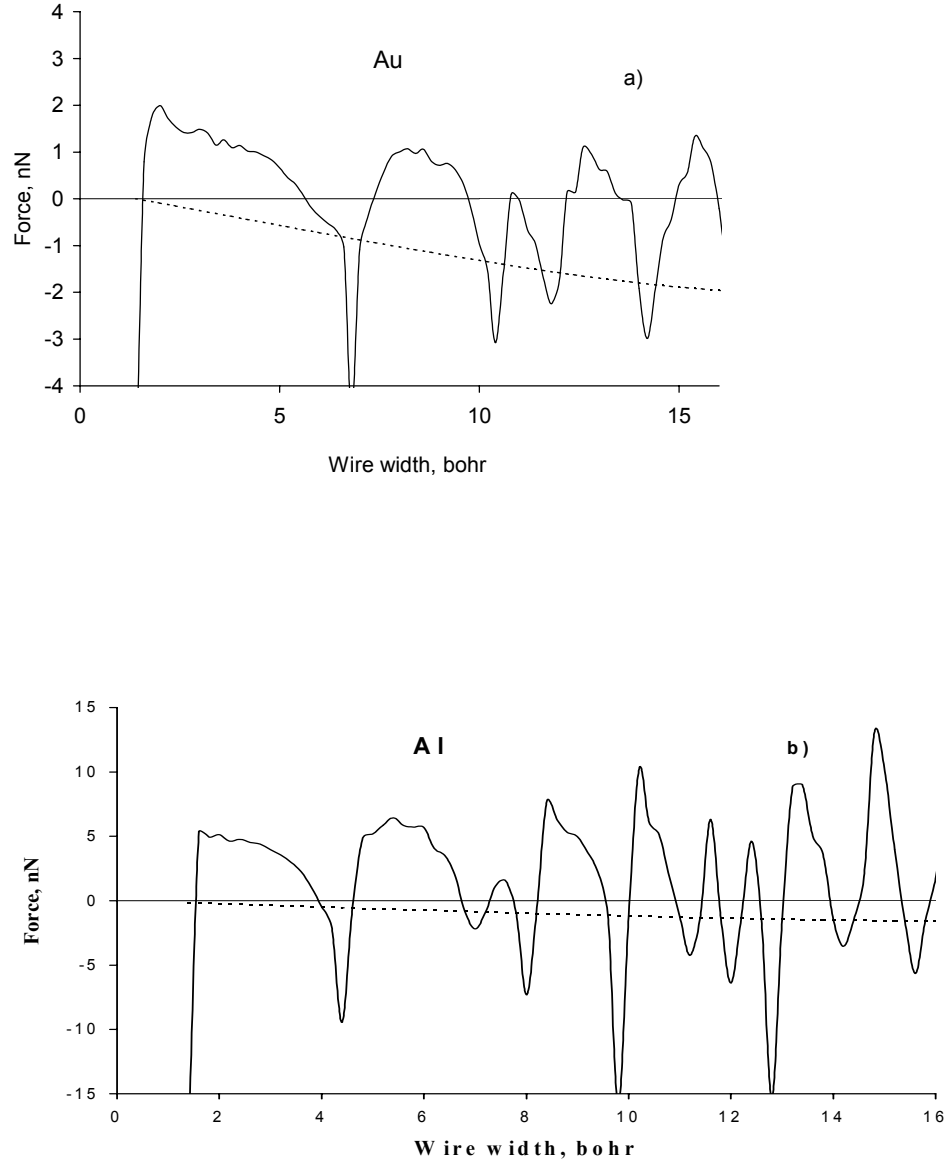


Fig.6. Force acting in the longitudinal direction of the Au and Al wires (solid curve). The dashed curve indicates the contribution to the force due to the macroscopic surface tension.

The total kinetic energy K_e of electrons in the finite wire needed to determine the elongation force was calculated from (23). The monotonic component of $K_e(a)$ decreases with an increase of the wire width and approaches well-known asymptotic value $\frac{3}{5}NE_F^0$. As already discussed, in formula (27) this dependence appears with an opposite sign compared to that for wire with a fixed Fermi level in a point contact [5]. To calculate the surface energy component we have employed the experimental values of surface tension $\sigma = 1500, 1180$ erg/cm² for Au and Al, respectively. Then, applying Eq.(27), we calculate the force fluctuations. They are expressed in nanoNewtons and plotted in Fig.6 for Au and Al whiskers.

The amplitudes of fluctuations in gold whisker are similar to those measured for gold point contacts (about 2nN). As can be seen from Fig.6, for a given volume Ω and shape of the surface, the surface contribution to the elongation force is small. This agrees with the results of more sophisticated density-functional calculations for infinite cylindrical wires [12].

Finally, let us note that in reality the shape of wire does not have a definite radial symmetry. On the other hand, the hierarchy of stationary levels can be fixed accurately only for a sample of simple symmetry. Therefore the usage of a cuboidal enclosure to represent a nanowire appears to be quite reasonable.

Possibly the practical usage of quantum whiskers is in the atomic-sized switches or high sensitive pick-up of vibration. The results presented in this paper are useful for investigation of physical process in the various types of the field-emission structures with the tip radius less than 10^3 bohrs and surface crystallites of atomic size. There are needle cold cathodes, arrays and so on, which can be used as efficient electron sources [30-32]. The results obtained permit is to investigate and to choose in practice more suitable emitter characteristics to improve the reliability of the electronic devices. As to metals and semiconductors, a possible influence of the finite dimensions on the field emission characteristics has not been investigated yet.

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