Electron and Positron States in Layered Metal/Dielectric Nanostructures

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(Received 14 July 2016; published online 29 November 2016)

Within the framework of modified Kohn-Sham method and stable jelly model with taking into account image forces and conduction band profiles of the dielectric, self-consistent calculations of potential profiles, the work functions and Schottky barriers for asymmetric metal-dielectric film systems, in which dielectrics on both sides of the metal nanofilms are different, were performed. Dielectric environment generally leads to negative changes in the electron work function and surface energy. In view of the dielectric conduction band (solid inert gases, SiO₂), the size effects, the impact of effective mass on energy and annihilation characteristics of positrons in layered structures with self-consistent hybrid potential profiles built in the local density approximation and crosslinked with image potentials were investigated. The possibility of localization of a positronium atom in nanosandvich was discussed. Comparison with the experiments was done.

Keywords: Metal nanofilm, Electronic states, The metal-dielectric contact, The Schottky barrier, Density functional method, Positron states, Annihilation characteristics.

DOI: 10.21272/jnep.8(4(1)).04050

PACS numbers: 73.30. + y, 71.60. + z

1. INTRODUCTION

Studies of metal films on semiconductor or dielectric substrates, in addition to the fundamental objectives, set the task of creating new nanoscale devices. A comparatively small number of experimental works aimed at the quantum-size effects ([1-5] and references therein) indicates the complexity of obtaining measurement objects and methods necessary for the study. It should be noted that metal films are deposited on different substrates, but until now, apart from a small number of works [4], the methods of self-consistent calculations are developed only for hypothetical metal films in vacuum.

The electron work function is one of the important equilibrium characteristics of metal nanostructures. For a metal film on a dielectric substrate, it is necessary to introduce into the model information not only on its dielectric properties (constant ϵ), but also about the conduction band bottom depth (– χ_e) with respect to the vacuum level (χ_e is the electron affinity). The neglect of the conduction band of electrons is one of the approximations. This approach ($\chi_e = 0$) was used to calculate the work function, polarization and surface plasmon resonance in nanoclusters and wires located in different dielectric matrices (see, for example, [6, 7] and references therein).

When the electron escapes from the metal, it is accompanied by the exchange-correlation hole, which is localized and spread over the mirror image surface taking the view of the mirror image charge. This representation does not correspond to the local density approximation (LD), which is the basis of self-consistent calculations of the exchange-correlation energy of heterogeneous manyelectron systems. The mirror image potential in this approximation does not coincide with the expression of classical electrodynamics.

Multiple attempts to calculate the mirror image potential within the Kohn-Sham method did not lead to a satisfactory result (see, for example, [8]). However, in [9], a comparatively simple approach was proposed to overcome this complexity, staying in the framework of a selfconsistent procedure. This approach is used in this paper.

Slow positron beams are used to diagnose the structure of solids, nano-objects, also by applying a positron microscope. Electron-positron annihilation gives unique information on the bulk and surface electronic structure [10-12], point defects of pure materials and their oxides [13, 14], as well as ceramics [15] and nanostructures [16]. Injected positrons in the near-surface region of metals and their oxides [17-19] are capable of forming positronium (Ps) atoms with the exciton-like spectrum.

Some interest in the literature is also devoted to the determination of the binding energy and lifetime of P_s atoms near the silica surface [20-23], the study of positron transport in the metal-oxide-semiconductor systems [24, 25] and also of solid inert gases used as moderators for positron beams.

The experimental detection of the P_{S_2} molecule in Si nanopores is reported in [26], and in [27] – the formation of exciton droplets in cooled GaAs under the action of laser pulses that makes attractive the search for conditions and structures for condensation of P_S and electron-positron clusters [28].

The aim of this work is to calculate the energy characteristics of a metal film in contact with dielectrics, as well as spectral and annihilation characteristics of positrons injected into metal-dielectric layered structures.

2. ENERGY CHARACTERISTICS OF ELECTRONS AND POSITRONS

2.1 Statement of the problem

Let us consider a metal film of thickness L at zero temperature and direct the *z*-axis perpendicular to the film plane (see Fig. 1).

For conduction electrons of the metal film, the thickness *L* of which is of the order of the Fermi wavelength and much smaller than its other dimensions ($L \ll L_x, L_y$), the variables in the three-dimensional wave equation are separated, the electron motion along the *x* and *y* axes is described by plane waves, and the corresponding compo-

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nents of the wave vectors are continuous. The components of one-electron wave functions $\psi^{e}(z)$ correspond to the motion, which is normal to the surface (with the energy of the electron "subband" ε^{e}_{a}).

The calculation technique is the following: first, all the characteristics of electrons in such a system are calculated in the absence of positrons: electron spatial distribution profiles, electron potential profiles, electron work function and Schottky barriers. Dielectrics on both sides of the metal film (see Fig. 1) are modeled by the dialectric constants ϵ and the electron conduction band bottom depths (– χ_e) with respect to the vacuum level.

Then, a positron is placed in such a system. The electron spatial distribution profiles, which have been already calculated (in the absence of the positron), are used to determine the electron-positron contribution to the functional, and then – for the effective potential containing positron. Now, the dielectrics on both sides of the metal film are modeled for the positron not only by the dielectric constants ϵ , but also the positron conduction band bottom depths (– χ_{ρ}) with respect to the vacuum level. As a result of the solution of the Schrödinger wave equation, the wave functions $\psi^e(z)$, positron spatial distributions and ε^{ρ}_j (the energy of the *j*-th surface positron subband) are determined.

2.2 Calculation of the effective potential, surface energy, electron work function and Schottky barrier

The distribution of a positive (ionic) charge is modeled by the following step function:

$$\rho(z) = \overline{n}\theta\left(\frac{L}{2} - |z|\right). \tag{1}$$

The one-electron wave functions $\psi^e_i(z)$ corresponding to the motion normal to the surface (with the "subband" energy ε^e_i) are found by the self-consistent solution of the system of the Kohn-Sham equations with the effective potential

$$v_{\text{eff}}^{e}\left[z, n(z)\right] = \varphi(z) + v_{xc}^{e}(z) + \langle \delta v \rangle_{WS} \theta\left(\frac{L}{2} - |z|\right)$$
(2)

and the Poisson equation

$$\nabla^2 \varphi(z) = -\frac{4\pi}{\epsilon(z)} \Big[n_e(z) - \rho(z) \Big]$$

in which the step function is used

$$\epsilon(Z) = \begin{cases} 1; & z < -L/2, -L/2 < z < L/2, z > L/2, \\ \epsilon_{1}; & -L/2 < z < -L/2, \\ \epsilon_{r}; & L/2 < z < L/2. \end{cases}$$
(3)

Here ϵ_l and ϵ_r are the dielectric constants of the dielectrics to the left and to the right of the film, respectively. The exchange-correlation potential $v_{xc}^e(z)$ is used in the LD approximation.

Applying to the metal-dielectric sandwiches (Fig. 1) the approach with taking into account the mirror image forces [9], we can write



Fig. 1 – Geometric film scheme in the dielectric environment

$$V_{\rm xc}^{\circ}(Z) = \begin{cases} V_{\rm xc}^{\rm NL,r}(Z), & Z \le Z', \\ V_{\rm xc}^{\rm LD}(Z), & Z' \le Z \le Z', \\ V_{\rm xc}^{\rm NL,r}(Z), & Z \ge Z'', \end{cases}$$
(4)

where $Z' = -L/2 - z_0'$, $Z' = L/2 + z_0'$ are the positions of the image planes ($z_0^{l,r} > 0$ are counted from the left and right boundaries of the film of thickness *L*);

$$v_{\rm xc}^{\rm NL,l} = -\chi_e^{\ l} + \frac{1 - \left[1 - \left(z - Z^{l}\right) / \left(4\lambda_l\right)\right] e^{\left(z - Z^{l}\right) / \lambda_l}}{4\epsilon_l \left(z - Z^{l}\right)}, \quad (5)$$

$$v_{xc}^{\text{NL},r} = -\chi_e^r - \frac{1 - [1 + (z - Z^r) / (4\lambda_r)]e^{-(z - Z^r) / \lambda_r}}{4\epsilon_r (z - Z^r)}.$$
 (6)

For example, expression (6) at $z \to \infty$ has the asymptotics $\left\{-\chi_e^r - \left[4\epsilon_r \left(z-Z^r\right)\right]^{-1}\right\}$ – the image potential (here $e = \hbar = m = 1$).

Under the condition of continuity of the potential (4) and its derivatives in the points $z = Z^{l}$, Z^{r} , we obtain the following relationships:

$$\lambda_{l,r} = -\frac{3}{16\epsilon_{l,r} \left[V_{\rm xc}^{\rm LD} \left(Z^{l,r} \right) + \chi_e^{l,r} \right]}, \tag{7}$$

$$\frac{\left| dV_{xc}^{LD} / dZ \right|_{Z=Z^{l,r}}}{\left[V_{xc}^{LD} \left(Z^{l,r} \right) + \chi_{e}^{l,r} \right]} = \frac{16}{9} \epsilon_{l,r} .$$
(8)

The expression (8) is used as the equation for finding $z_0^{I,r}$. The values of $z_0^{I,r}$ to the left and to the right of the film are calculated at each iteration by the solution of the Kohn-Sham equations. It should be reminded that $v_{xc}^e(z)$, as well as the electrostatic potential $\varphi(z)$, are the components of the effective (Coulomb) potential $v_{eff}^e(z)$. Thus, the effective potential is self-consistently crosslinked with the mirror image potential, which is accurate at large distances from the metal film surface, on both sides of the metal nanofilm.

The electron density profile $n_e(z)$ is expressed by the wave functions $\psi^e_i(z)$

$$n_{e}(z) = \frac{1}{2\pi} \sum_{i=1}^{i_{F}} k_{F(i)}^{2} \frac{\left|\psi_{i}^{e}(z)\right|^{2}}{C_{i}^{2}},$$
(9)

where the coefficients $C_i^2 = \int_{-\infty}^{+\infty} dz |\psi_i^e(z)|^2$;

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$$k_{\mathsf{F}(i)}^2 \equiv 2\left(\varepsilon_{\mathsf{F}} - \varepsilon_i^e\right); \tag{10}$$

 $i_{\rm F}$ is the number of the last occupied or partially occupied electron subband. The values of $i_{\rm F}$ and $\varepsilon_{\rm F}$ are determined by the solution of the equation

$$i_{\mathsf{F}}\varepsilon_{\mathsf{F}} = \pi L \overline{n}_e + \sum_{i=1}^{i_{\mathsf{F}}} \varepsilon_{i_i}^e \cdot \varepsilon_{i_{\mathsf{F}}} \le \varepsilon_{\mathsf{F}}; i = 1, 2, \dots, i_{\mathsf{F}}, \quad (11)$$

which follows from the definition for the Fermi energy and the normalization conditions.

Friedel oscillations in the nanofilms are significant throughout the bulk, therefore, the energies are counted from the vacuum level (this is the electron rest energy in the range of $|z| \gg L/2$). For the coupled states, the energies are negative for $\varepsilon_{\rm F}$, etc.

We apply this approach for three samples with "perfect" interfaces: Al films on SiO₂ and Al₂O₃, as well as SiO₂/Al/Al₂O₃ sandwich. They are designated in [29] as $\{1|AI|\epsilon_r\}$ and $\{1|AI|\epsilon_l\}$. For them, we use the following values of $\chi_e^{l,r}$ from Table 1 for the metal/vacuum interface: $\chi_e^{l} = 0$ and $\epsilon_l = 1$.

Table 1 – Examples of materials of the simplest coatings or substrates [30]

Materials	He	Ne	Ar	Kr	Xe	SiO ₂	AI_2O_3
ϵ	1.10	1.20	1.50	1.65	1.90	4	9
$\chi_{e'} \mathrm{eV}$	- 1.0	0.10	0.20	0.45	0.68	1.1	1.35

Accounting of the dielectric conduction band requires correction of the electron work function of the film: unlike the work function for the film in vacuum

$$W = -\varepsilon_{\rm F} \,, \tag{12}$$

the work function for the film in dielectric environment

$$W_d^{l,r} = -\varepsilon_{\rm F} - \chi_e^{l,r}.$$
 (13)

The value of W_d characterizes the Schottky barrier (i.e. the potential barrier height at the metal/dielectric interface), the measurement techniques of which are well-known [2, 30]. The possible cases of contacts of different materials: $|\varepsilon_{\rm F}| > \chi_e^{Lr}$ and $\leq \chi_e^{Lr}$. It should be noted that in formulas (12), (13), the values of $\varepsilon_{\rm F}$ differ from each other if they are calculated for one film, but in different environments.

2.3 Binding energy and lifetime of positrons

We place in this structure a positron, whose state is described by the effective potential

$$v_{\text{eff}}^{\rho}\left(z\right) = -e\varphi\left(z\right) + E_{0}\theta\left(\frac{L}{2} - \left|z\right|\right) + v_{\text{cor}}^{\rho-e}\left(z\right), \quad (14)$$

where the distributions $n_e(z)$ and $\phi(z)$, which are not deformed by this positron, are used; that is, $\phi(z)$ in the expressions (2) and (14) are the same. Competition of the terms in (14) leads to the fact that the potential wells for the positron are realized at the contact boundaries.

Positron-electron correlation interaction is defined as

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$$V_{\text{cor}}^{\rho-e}(Z) = \begin{cases} -\chi_{\rho}^{\prime} - \frac{e^{2}}{4\epsilon_{\ell}(Z^{\prime} - Z)}, & Z \leq Z_{\text{cut}}^{\prime}, \\ V_{\text{cor},\text{LD}}^{\rho-e}(Z^{\prime}), & Z_{\text{cut}}^{\prime} \leq Z \leq Z^{\prime}, \\ v_{\text{cor},\text{LD}}^{\rho-e}(Z), & Z^{\prime} \leq Z \leq Z^{r}, \\ v_{\text{cor},\text{LD}}^{\rho-e}(Z^{r}), & Z^{r} \leq Z \leq Z_{\text{cut}}^{r}, \\ -\chi_{\rho}^{r} - \frac{e^{2}}{4\epsilon_{r}(Z - Z^{\prime})}, & Z \geq Z_{\text{cut}}^{r}, \end{cases}$$
(15)

where $Z' = -L/2 - z_0'$, $Z^r = L/2 + z_0^r$ are the positions of the image planes ($z_0^{l,r} > 0$), $v_{\text{cor,LD}}^{p-e}(z)$ is the potential calculated in the LD approximation [31]. The expressions for the truncation radii have the form

$$Z_{\text{cut}}^{l,r} = \frac{\pm e^2}{4\epsilon_l \left[V_{\text{cor,LD}}^{\rho-e} \left(Z^{l,r} \right) + \chi_p^{l,r} \right]} + Z^{l,r}$$

where the signs + and – relate to Z_{cut}^{l} and Z_{cut}^{r} , respectively. The image forces for the electron and positron, in accordance with the classical electrodynamics, should be the same. Therefore, we assume that the positions of their image planes will also be the same. As a result, the values of $z_0^{l,r}$ for $v_{cor}^{p-e}(z)$ are identical to those calculated for $v_{xc}^e(z)$.

The positron intrinsic energy is written as

$$\varepsilon_{jk_{\parallel}}^{p} = \varepsilon_{j}^{p} + \frac{\hbar^{2}k_{\parallel}^{2}}{2m_{p}}, \quad k_{\parallel}^{2} = k_{x}^{2} + k_{y}^{2},$$
 (16)

where ε_j^{p} is the energy of the *j*-th surface positron subband, to which the wave function $\psi_j^{p}(z)$ corresponds.

For the positron, the Schrödinger equation is solved using the transfer T-matrix [32], which couples the waves incident on the barrier right-to-left and left-to-right. To this end, the range of heterogeneity of the potential profile $v_{eff}^{\rho}(z)$ was divided into $N \approx 10^3$ parts, in each of which the potential was considered constant.

The positron annihilation rate λ is determined by the sum of the annihilation rates in a metal plate λ^{AI} and in dielectrics λ^{d} ($\lambda^{AI} = \lambda^{d}$) due to the absence of intrinsic free electrons in the dielectric. Therefore, the positron lifetime in nanosandwiches $\tau = \lambda^{-1}$ is determined only by one-dimensional distributions of conduction electrons of

a metal film $n_e(z)$ and a localized positron $n_i^p(z) = |\psi_i^p(z)|^2$

$$\pi_j^{-1} = \pi r_0^2 c \int dz n_e(z) n_j^p(z) \Gamma\left(n_e(z)\right), \qquad (17)$$

where r_0 is the classical electron radius, c is the light speed, Γ is the extension factor for the positron in quasihomogeneous electron gas of concentration $n_e(z)$.

2.4 Influence of effective masses on positron states in metal/dielectric nanosandwiches

Let us evaluate the influence of effective masses on the calculated characteristics, for example, for the system vacuum/Al/SiO₂. For such a system, $\epsilon_I = 1$, $\chi_e^{\ I} = \chi_p^{\ I} = 0$.

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Accounting of the effective mass will be carried out by analogy with that as usual in heterostructures [33].

In the vacuum range (z < -L/2), $m_p^* = m_e^* = m$, m is the free electron mass.

In [34], the values of the effective mass $m_p^* = 1.15 m$ are calculated for metals with a cubic lattice, and in [35], the values $m_p^* = 1.5 m$ are used for all solids. In the case of metal nanofilms, the use of the value $m_p^* = m$ (if we are talking about single positrons) is justified for the calculation of the ground state energy. The reasons for this choice are the following. To calculate the surface subband energies $\varepsilon_{\!\!j}^{\rho}$, a one-dimensional wave equation along the z-axis with the corresponding component of the effective mass tensor should be solved. Due to the fact that the greatest interest is in the films with a thickness of several monolayers (ML), i.e. with a thickness much smaller than the positron mean free path, in the range of -L/2 < z < L/2 we choose $m_p^* = m_e^* = m$. In the x and y directions, the mass tensor components, different from m, influence only the positron density of states, but not on the subband energies.

The effective mass of the positron m_p^* in SiO₂ was defined by the effective mass of the positronium atom $M_{P_s}^* = m_e^* + m_p^*$. Based on the empirical data in [36] and estimates in [37], $M_{P_s}^* = 2.84m$. In the range of z < L/2, using the value $m_e^* = 0.42m$ recommended in [38], we have $m_p^* = 0.42m$. In order to test these values, we can define the binding energy of P_s in the volume of SiO₂

$$E_B = \frac{\text{Ry}}{\varepsilon^2} \frac{m_e m_p^*}{m_e^* + m_p^*}, \quad \text{Ry} = 13.6 \text{ eV}.$$

The obtained value $E_B = 0.304 \text{ eV}$ is approximately 2 times larger than the experimental one [20] calculated in [23] for P_S on the surface of SiO₂.

It should be noted that as a result of the introduction of the effective electron mass, the "electronic" part of the problem, i.e. the potentials (2) and (14), is recalculated.

3. RESULTS AND DISCUSSION

3.1 Calculation results of the sandwich characteristics in the absence of the positron

In the model, the following parameters are specified: r_s is the average distance between the conduction electrons of the metal, the values ϵ and χ_e of the dielectric. The values λ and z_0 are calculated self-consistently in the framework of the Kohn-Sham procedure. Therefore, for a particular metal, all its electronic characteristics are the functions of ϵ and χ_e .

The Kohn-Sham equations (with taking into account the formulas (4)-(7)), together with the Poisson equation, were solved by numerical methods for the stable jelly model of the metal film in the dielectric environment [29]. As an illustration, in Fig. 2 we present the calculation results of the potential profiles.

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Fig. 2 – Electrostatic, exchange-correlation and effective potential profiles for vacuum/Al(111)/Al₂O₃ and SiO₂/Al(111)/Al₂O₃ sandwich. Film thickness L = 3 ML. The circles indicate the coordinates of crosslinked nonlocal and local potentials

To answer the question, if the values of $\chi_e^{l,r}$ are the variation parameters, the calculations are performed at $\chi_e^{l,r} = 0$ for all three structures. It is found that neither the behavior of the potential ν_{xc}^e inside the film, nor the position of ε_{F} do not actually depend on the modernization of ν_{xc}^e . Only the parameters $z_0^{l,r}$, $\lambda^{l,r}$ and the well wings depend significantly on such manipulations. In general, the behavior of $\nu_{eff}^e(z)$ out of the well is caused not only by the presence of the conduction band ($\chi_e \neq 0$) in the dielectric, but also by the non-locality of ν_{xc}^e .

It was also revealed that the use of the nonlocal exchange-correlation potential in the iterative procedure leads to a significant suppression left in vacuum of the potential hump in the effective (but not in the electrostatic) potential (Fig. 2). The presence of such a hump was detected in [20].

In Table 2 we present the calculation results for three samples from Al(111) nanofilm (with thickness *L* in ML; 1ML = 4.4 a_0 for Al(111)). The calculations are also performed for unbounded systems ($L = \infty$): $W_d^r = 1.84$ and 1.29 eV for Al/SiO₂ and Al/Al₂O₃, respectively. However, these calculations do not take into account the presence to the left of the metal-vacuum interface. Therefore, the comparison of these values with the data of Table 2 is incorrect, since the result depends on the average value of the dielectric constant $\langle \epsilon \rangle = (\epsilon_1 + \epsilon_2)/2$, and not only on the value of ϵ_r [29].

The obtained results indicate the possibility of controlling the Schottky barrier, variation of the metal film thickness (in technologies, the oxide thickness is a tool to control the effects in the channel).

Table 2 – Calculation results for Al films on SiO₂ (the upper value), for Al films on Al₂O₃ (the middle value) and for the sandwich SiO₂/Al(111)/Al₂O₃ (the lower value)

L, ML	z_0^\prime , a_0	Z_0^r , a_0	λ' , $a_{_0}$	λ^r , a_0	W_d^\prime , eV	W_d^r , eV	γ, erg/cm ²
1	1.05	3.35	0.977	0.706	3.43	2.33	821
	1.00	4.25	0.962	0.518	3.01	1.66	760
	3.30	4.15	0.707	0.519	1.79	1.54	607
2	0.95	2.85	0.946	0.643	3.26	2.16	755
	0.95	3.60	0.945	0.474	2.84	1.49	704
	2.85	3.60	0.640	0.479	1.62	1.37	548
3	0.85	2.60	0.921	0.606	2.94	1.84	734
	0.85	3.50	0.919	0.476	2.63	1.28	696
	2.95	3.80	0.672	0.512	1.56	1.31	562
4	0.90	3.05	0.933	0.683	3.23	2.13	779
	0.95	4.05	0.948	0.531	2.86	1.51	735
	3.10	4.05	0.688	0.535	1.69	1.44	578
5	0.90	2.95	0.932	0.661	3.23	2.13	764
	0.95	3.85	0.948	0.507	2.84	1.49	716
	3.00	3.85	0.671	0.512	1.65	1.40	556
6	0.90	2.85	0.934	0.651	3.13	2.03	751
	0.90	3.65	0.933	0.489	2.73	1.38	705
	2.85	3.65	0.645	0.491	1.54	1.29	550
7	0.90	2.95	0.934	0.669	3.17	2.07	770
	0.90	3.90	0.933	0.520	2.80	1.45	726
	3.05	3.95	0.684	0.527	1.65	1.40	569

For the auto-field emission current, as in the Fowler-Nordheim model, the spatial profile of the effective potential, which is added to the external electrostatic potential $\phi_{\text{ext}}(z)$ starting from the points $z = Z^{l,r}$, is a determining factor.

Let us compare with the experimental data. The calculated value of the work function of the AI(111)/vacuum face is equal to 4.12 eV, experimental ones for AI(111) – from 3.11 ± 0.10 to 4.26 ± 0.03 eV, and for polycrystal-line AI – 4.28 eV [39].

The Schottky barrier for Au/Al₂O₃ measured in [40] is 3.5 ± 0.1 eV. We note that the experimental values of the work function of Au and Al in [39] are identical.

On the other hand, the Schottky barrier measured in [41] for AI, Ag, Cu on a thin (of 35 nm thick) Al₂O₃ film is equal to 1.66; 1.72; 1.80 eV. This is in agreement with the value 1.5 eV for Al/Al₂O₃ in [30]. W_d = 3.19 eV is also recommended for Al/SiO₂ in [30].

The value of $W_d = 0.5...0.8$ eV for 15 metals deposited on Si should be referred to the mode $|_{\mathcal{E}_F}| \le \chi_e^{l,r}$ [30]. In [41], the measured barrier height varied from 0.6 to 0.49 eV with increasing Ti/Si film thickness from 50 to 90 nm. As seen, the measurement data are ambiguous.

Note that the introduction of the nonlocal potential does not significantly influence the position of the Fermi level in a metal film contacting with the dielectric.

Accounting of the conduction band in the dielectric and the self-consistence of the well shape for the film electrons changes the spectrum (number of subbands) and the density of states, and, thus, the magnitude of the optical transition matrix elements and the optical absorption coefficient [42]. The equilibrium profile of electrons and electrostatic potential is necessary to calculate the auto-field emission of electrons and annihilation characteristics of positrons in nanostructures.

3.2 Calculation results of the positron states

 ϵ_r , χ_e^r and χ_p^r are the initial parameters for the calculations: the values of ϵ_r and χ_e^r for the dielectrics utilized are given in Table 1 and $\chi_p^r = (0.6; 1.55; 2; 2.3) \text{ eV}$ for Ne, Ar, Kr, Xe, respectively, are taken from [19].

Since the experimental value of χ_p for SiO₂ is not known, we evaluated it using the Born cycle

$$\chi_{\rm Ps} - \chi_e - \chi_p + \frac{Ry}{2} = 0 ,$$

where χ_{Ps} is the positronium atom work function of SiO₂ into vacuum. As an assumption here it is suggested that the electron in SiO₂ is at the conduction band bottom. Using for SiO₂ the experimental values of the work functions $\chi_{Ps} = -3.27 \text{ eV}$ [23] and $\chi_e = 1.1 \text{ eV}$, we obtain $\chi_p^r = 2.43 \text{ eV}$.

In Fig. 3 we illustrate the spatial distributions of the positron potential components for AI films of a thickness of L = 1 and 3 ML. The solid lines correspond to the self-consistent calculations done under the assumption that $m_e = m_p = m$, the dotted lines – $m_e^* = 0.42m$, $m_p^* = 2.42m$ in the SiO₂ range.

Due to the fact that the potential distribution $\phi(z)$ in the vacuum region (z < L/2) has a maximum (potential hump [29]), the dependence – $\phi(z)$, respectively, should have a minimum, as observed in Fig. 3. Its depth increases with increasing difference between the values of ϵ_I and ϵ_r and with increasing film thickness *L*.

It is interesting to compare the obtained values with the calculation results for the aluminum/vacuum contact ($\tau_1 = 334$ ps). The difference is tens of picoseconds at an experimental measurement accuracy of 1 ps.

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Fig. 3 – Self-consistent profiles of the electrostatic (with the opposite sign), correlation and effective potentials of the positron, as well as its spatial distribution $|\psi_j^p(z)|^2$ for vacuum/AI(111)/SiO₂ film. *j* is the subband number. Al film thickness is 1 and 3 ML. The dotted lines indicate the profile obtained taking into account the effective masses



Fig. 4 – Size dependences of the positron subband energies and lifetimes for vacuum/Al(111)/SiO₂ film. The dotted lines indicate the profile obtained taking into account the effective masses

Fig. 5 contains information for vacuum/Al(111)/solid inert gases structures similar to that presented in Fig. 4 for j = 1 and 2 under the condition $m_e = m_p = m$.

The doublet of states for these dielectrics is less pronounced; however, the size dependence of the lifetimes is more significant than that in Fig. 4. For film thicknesses L > 1 ML and at a contact with Ne, Ar, Kr and Xe, the values of τ_j differ by about 10 ps. If the film is placed between two dielectrics, then the calculation results will be determined by the competition between characteristics of dielectrics and AI, and hardly undergo fundamental changes. The barrier height between two wells depends on the metal type. If substitute AI, for example, by Na, the barrier actually disappears, and the wells are united.



Fig. 5 - Size dependences of the positron subband energies and lifetimes for AI(111)film in contact with solid inert gases

We also note that when a current flows in imperfect metal-dielectric contacts, a part of external electrons is trapped near the metal surface. The potential generated by them will further facilitate localization of positrons.

The calculations of the work function of the positronium atom into vacuum W_{Ps} were also performed, for example, for vacuum/AI(111)/SiO₂ system, using the Born cycle: $W_{Ps}(L) = W_e(L) - \varepsilon_l^p(L) - Ry/2$. Here, $W_e(L)$ is the electron work function for the same system in the absence of the positron. Taking into consideration Table 1, we obtain $W_e(L) = 3.43$; 3.26; 2.94; 3.17 eV for L = 1, 2,3, 7 ML, respectively. The calculated values of the positron ground state energies $\varepsilon_l^p(L)$ are illustrated in Fig. 4. After the substitution, we have $W_{Ps}(L) = +0.25$; -0.08; -0.45; -0.16 eV for L = 1, 2, 3, and 7 ML, respectively. It should be recalled that if $W_{P_c}(L) > 0$, then the Ps atom is localized in the system, as for the case when L = 1. The comparison of the value of W_{P_s} for L = 1 ML with the experimental value of the work function $\chi_{P_s} = -3.27 \text{ eV}$ [20] for vacuum/SiO₂ indicates that the positronium is locked from the side of SiO₂. These estimates are made under the assumption $m_{p}^{*} = m_{e}^{*} = m$. The introduction of

effective masses $m_e^* \neq m$ and $m_p^* \neq m$ makes possible localization for any values of *L*.

Thus, it is possible to make an optimistic conclusion about the ability of metal-dielectric nanosandwiches to condense the positronium atoms.

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atoms in the surface potential can also be expected for thee clusters of metals embedded in dielectric matrices by analogy with quantum dots [43].

4. CONCLUSIONS

The method of self-consistent calculations of the characteristics of a metal film in dielectrics is proposed in the paper. The case of asymmetric metal-dielectric sandwiches - different dielectrics on both sides of the film - is considered in the framework of the modified Kohn-Sham method and the stable jelly model. Taking into account the image forces and conduction band of the dielectric, the potential, electron work function and Schottky barrier profiles are found for aluminum nanofilms with perfect vacuum/AI(111)/SiO₂, vacuum/AI(111)/AI₂O₃ interfaces and SiO₂/AI(111)/AI₂O₃ sandwich. The dielectric environment in general leads to a decrease in the electron work function and surface energy. In addition to size oscillations, the change in the electron work function is determined by the arithmetic mean value of the dielectric constants on either side of the metal film.

The self-consistent calculations of the potential, wave function, surface subband energy and lifetime profiles of positrons are performed for AI nanofilms, which are in contact with dielectrics (solid inert gases, SiO₂). The size effects, the influence of effective masses of electrons and positrons on energy and annihilation characteristics in systems with double potential wells caused by the image potentials are investigated. The possibility of localizing the positronium atom in nanosandwiches is discussed.

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