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Spectroscopy of positronium in nanomaterials

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ABSTARCT

The theory of positronium states in a spherical nanopore localized in solid matrices is developed. Theoretical researches are carried out in energy spectrum and binding energy of positronium in a nanopore and their dependences on the nanopore radius a under conditions of contributing largely the polarization interaction of positronium with a spherical "nanopore-matrix" interface. The question is discussed connected with the possibility of experimental observation of the states of positronium localized in a nanopore. The new method is proposed for optical spectroscopic determination of nanopore sizes a in materials, based on comparison of experimental absorption (radiation, reflection) spectra of positronium in nanopores with theoretical dependences of energy spectra of positronium on radius a of nanopores.

Key words*:* parapositronium states, energy spectrum of positronium, binding energy of positronium, Coulomb and polarization interaction, optical spectra, nanopores

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INTRODUCTION

At present the phenomenon of electron-positron annihilation is being extensively used in physical researches. The effect of interaction of positrons with defects in matrices of inorganic and organic nature has been described in [1-4]. It was ascertained that positrons thermolyzed in the matrix bulk diffuse in the area of defects and capture by them. The interaction of positrons pointed out with electrons leads to annihilation with the radiation of energy quanta. As a result the possibility has been arisen to sound experimentally defects in matrices with the use of positrons. So, the method of electron-positron annihilation enables to investigate at the new level the state and electron structure of materials [1-4].

The expanse of interatomic distances connected with existing defects is inherent at the most to polycrystalline, amorphous, nanoporous, carcass, carbonic nanostructured materials [1-4]. The most effectively positrons is captured by the defects of free bulk type (vacancies, vacancy clusters, nanopores, vacancy-like defects in amorphous matrices and etc.), interlayer spaces in carbonic multilayer nanostructures [1-3]. In such systems every nanosized element pointed out has its characteristic specific structure of free bulk that can be investigated by the methods of electron-positron annihilation. This method is undestructive and characterized by high selectivity and sensitivity, the ability to find out pores at the surface and in the bulk of materials [1-4].

Using the method of annihilation of positrons it was found existing three-dimensional vacancy agglomerates (the nanopores of spherical shape) with radiuses $a \approx 100$ nm (and more up to micronic ones), with their sizes approximating to the crystallites of metals, as well as mineral (for instance, apatite-like) structures [3, 5-8]. Their linear sizes a are comparable with de Broyl wave length of quasi-particles (electron, positron and positronium) or (and) with Bohr radiuses of positronium. The latter circumstance leads to contributing largely the phenomena of spatial dimensional quantation of quasi-particles, in such nanosystems, into optical and electrooptical processes [5-8].

According to ideas [6-8], positronium is captured by a nanopore, or appears in its bulk. In making so it turns to be localized in a nanopore during all the time of its life. It is supposed also that diffusing in search of a free nanopore is not a positronium, but a positron. On meeting such a nanopore and interacting with a trek electron, positron forms positronium immediately in the nanopore bulk [7, 8].

Nowadays the properties of positronium in the nanopores of matrices have been studied insufficiently by experimental as well as theoretical methods. Therefore the investigations aimed at solving problems connected with the interaction of positronium located in the nanopores of matrices, with electromagnetic radiation, are actual with a scientific as well as a practical view.

In the present work the theory of positronium localized in a spherical nanopore of solid matrix is developed. Theoretical researches are carried out in energy spectrum and binding energy of parapositronium in a nanopore, as well as their dependence on the nanopore radius a under conditions of contributing largely the polarization interaction of positronium with a spherical "nanopore-matrix" interface. Also the question is discussed connected with the possibility to observe experimentally a positronium located in a nanopore. The new optical method is proposed to determine the sizes a of nanopores in materials, based on comparison of absorption (radiation, reflection) spectra of positronium in nanopores with theoretical dependences of energy spectra of positronium on radius a of nanopores.

The paper is organized as follows. In Section 2 we discuss the energy spectrum of positronium states. In section 3 we consider absorption spectra of light by the positronium states in the nanopores of solid matrices.

MATERIALS AND METHODS

The energy spectrum of positronium in a nanopore

Let us consider the model of quasi-zero-dimensional system: a neutral dielectric spherical nanopore with radius a, filled with dielectric medium (with permittivity ε_1), surrounded by dielectric matrix (with permittivity ε_2). In the bulk of such nanopore motions can be carried out by electron e, positron p with effective masses m_e и m_p, so as $m_e=m_p=m_0$; and also by positronium with its resulted effective mass $\mu=(m_0/2)$ (where m_0 – the mass of electron in vacuum, r_e and r_p – the distances of electron and positron from the center of nanopore (Fig. 1). The characteristic sizes of the problem are the values a, a_e, a_p, a_{ep}, where

$$a_e = a_p = \frac{\hbar^2 \varepsilon_2}{m_0 e^2}, \qquad a_{ep} = \frac{2\hbar^2 \varepsilon_2}{m_0 e^2} \qquad (1)$$

— the Bohr radiuses of electron, positron and positronium, respectively, in dielectric medium (with permittivity ε_2). A nanopore radius being considerably larger than the Bohr radius value of positronium a_{ep},

$$a >> a_{ep} \qquad (2)$$

one can consider the motion of electron and positron in a nanopore with approximation of effective mass [4,5].

The energy of polarization interaction $U(\mathbf{r_e},\mathbf{r_p},a)$ of electron and positron with a spherical "nanopore-matrix" interface can be introduced as the algebraic sum of the energies of interaction of positron and electron with their own $V_{pp'}(r_p,a)$, $V_{ee'}(r_e,a)$ (the "self-action" energy) and the "strange" $V_{pe'}(\mathbf{r_e},\mathbf{r_p},a)$, $V_{ep'}(\mathbf{r_e},\mathbf{r_p},a)$ images respectively [8,9] (Fig. 1):

$$U(\mathbf{r_e},\mathbf{r_p},a) = V_{pp'}(r_p,a) + V_{ee'}(r_e,a) + V_{ep'}(\mathbf{r_e},\mathbf{r_p},a) + V_{pe'}(\mathbf{r_e},\mathbf{r_p},a) \qquad (3)$$

Since the effective masses of electron m_e and positron m_p are equal to the mass of free electron m_0, it is energetically advantageous for positron and electron to locate in one straight passing through the center of a nanopore, and at the same distance $r_e = r_p = (\rho/2)$ (Fig. 1). In making so the energies of interaction $V_{pp'}(r_p,a)$, $V_{ee'}(r_e,a)$, $V_{ep'}(r_e,r_p,a)$, $V_{pe'}(r_e,r_p,a)$ can be written as:

$$V_{pp'}(\rho,S) = -\frac{E^{ep}}{S} \cdot \frac{1}{(1-\xi^2)}\beta \qquad (4)$$

$$V_{ee'}(\rho,S) = -\frac{E^0_{ep}}{S} \cdot \frac{1}{(1-\xi^2)}\beta \qquad (5)$$

$$V_{ep'}(\rho,S) = V_{pe'}(\rho,S) = \frac{E^0_{ep}}{S} \cdot \frac{1}{(1+\xi^2)} \qquad (6)$$

$$\beta = \frac{(\varepsilon_2 - \varepsilon_1)}{(\varepsilon_2 + \varepsilon_1)} \qquad (6a)$$

where β - the parameter of a nanosystem, the variable quantity $\xi = (\rho/2a)$. The energy of Coulomb interaction between electron and positron $V_{ep}(\rho)$ is described with such formula

$$V_{ep}(\rho) = -\frac{e^2}{\rho\varepsilon_2} \tag{7}$$

Here and then the energies are measured in the units

$$E_{ep}^0 = Ry_{ep} = \frac{m_0 e^4}{4\hbar^2\varepsilon_2^2} \tag{8}$$

where E_{ep}^0 – the binding energy of positronium in a nanopore and the nondimensional nanopore radius value is used $S = (a/a_{ep})$.

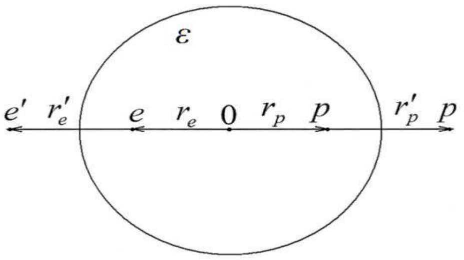

Fig. 1. The schematic image of positronium in a spherical nanopore. Radius vectors r_e и r_p determine the distance of electron e and positron p from the center (O point) of nanopore with radius a. The charges of images $e' = -(a/r_e)e$ and $p' = -(a/r_p)p$ are located in the distances $r_e' = -(a^2/r_e)$ and $r_p' = -(a^2/r_p)$ from the center of nanopore and represent point charges of the image of electron and positron respectively.

The potential energy of electron and positron moving in a nanopore of radius S,

$$U_{ep}(\rho, S) = U(\rho, S) + V_{ep}(\rho) \tag{9}$$

has a maximum in the point $r_e^0 = r_p^0 = r_0 = 0,48a$ (or at $\rho_0 = 0,96a$) and is equal to

$$U_{ep}^{\max}(\rho = \rho_0) = -3,057\,(E_{ep}^0/S) \tag{10}$$

In the quasi-zero-dimensional nanosystem model studied (Fig. 1), in the framework of approximations as stated above and also with the approximation of effective mass, and in the system of center of masses, the gamiltonian of positronium (parapositronium consisted of $1s$-electron and $1s$-positron with antiparallel spins) moving in the bulk of nanopore, can be written as:

$$H(\rho,a) = -\frac{\hbar^2}{2\mu}\cdot\frac{1}{\rho}\cdot\frac{d}{d\rho}\left(\rho\frac{d}{d\rho}\right) + V_{ep}(\rho) + V_{ep'}(\rho,a) + V_{pe'}(\rho,a) +$$

$$+V_{ee'}(\rho,a)+V_{pp'}(\rho,a)+V_e(\rho,a)+V_p(\rho,a) \qquad (11)$$

with the first part being the operator of kinetic energy of positronium, and the potentials

$$V_e(\rho,a),\ V_p(\rho,a) = \begin{cases} 0, & \rho \le 2a \\ \infty, & \rho > 2a \end{cases} \qquad (12)$$

describing the motion of quasi-particles in the bulk of nanopore with the help of endlessly deep potential hole model.

The gamiltonian of positronium (11) contains the energies of interaction of positron and electron with their own (4), (5) and the “strange” (6) images. The expressions describing the energies of interaction (4)-(6) were obtained in [4-6] in the framework of macroscopic electrostatics. Therefore the possibility of using the energies of interaction (4)-(6) in gamiltonian (11) can be justified if the nanopores studied have macroscopic sizes [8-11]

$$a \ge 2\ nm \qquad (12a)$$

In order to determine the energy spectrum of positronium $W(S)$ in a nanopore of radius S, one needs to solve Shredinger equation that in the system of center of masses and with approximation of effective mass, can be written as

$$-\frac{\hbar^2}{2\mu}\cdot\frac{1}{\rho}\cdot\frac{d}{d\rho}\left(\rho\frac{d\Psi(\rho,S)}{d\rho}\right)+H(\rho,S)\,\Psi(\rho,S)=W(S)\,\Psi(\rho,S) \qquad (13)$$

In the equation (13) gamiltonian $H(\rho,S)$ is determined by formulas (11) and (4) – (7), (12). The radial wave function of positronium (ρ,S) describes the relative motion of electron and positron in a nanopore of radius S.

The binding energy of positronium $E_{ep}(S)$, moving in a nanopore with radius S, is the decision of the radial Shredinger equation (13) with gamiltonian $H(\rho,S)$ containing (in contrast to gamiltonian (11)) only the parts

$$H(\rho,S) = -\frac{\hbar^2}{2\mu}\cdot\frac{1}{\rho}\cdot\frac{d}{d\rho}\left(\rho\frac{d}{d\rho}\right) + V_{ep}(\rho) + V_{ep'}(\rho,S) + V_{pe'}(\rho,S) \qquad (14)$$

Let us study the energy spectrum and the binding energy of parapositronium in a nanopore of radius S (2), (2a) by Wentzel-Kramers-Brillouin (WKB) method for free values of the principal quantum number n. In order to obtain from the condition of quantation, the boundary transition to the precise Coulomb spectrum of parapositronium

$$W_n = -\frac{E_{ep}^{0}}{n^2}, \qquad (15)$$

in the area of its applicability, for finding the phase in the quasi-classical wave function one needs to use the exact decision of Shredinger equation (13), with gamiltonian (11), at $\rho \to 0$. In making so the potential energy of electron-positron pare $U_{ep}(\rho, S)$ (9) looks as the Coulomb form (7). As a result one can obtain the quantation principle

$$S^{1/2}\int_{\xi_1}^{\xi_2} d\xi\,[-|\tilde{W}_n(S)|S + \left(\frac{1}{\xi} + \frac{2}{1-\xi^2} - \frac{2}{1+\xi^2}\right)]^{1/2} = \pi n, \tag{16}$$

where $\xi_{1,2}$ - the points of turn, the energy value $|\tilde{W}_n(S)| = |W_n(S)/E_{ep}^0|$. Leaving in the decomposition of potential energy of electron-positron pare $U_{ep}(\xi, S)$ (9) (with the parameter $\xi^2 \ll 1$) only the energy of Coulomb interaction between electron and positron (the part $\sim \xi^{-1}$), with the help of quantation principle (16) one can obtain the formula (15). The expression (15) describes the boundary transition of energy spectrum $W_n(S)$ of parapositronium to the exact Coulomb spectrum (15) in a nanopore of large radius *S*.

In analogy with formula (16), using the potential energy of electron-positron pare entered in gamiltonian (14), in order to determine the binding energy $E_{ep}^{(n)}(S)$ of parapositronium one can obtain the quantation principle as follows:

$$S^{1/2}\int_{\xi_1}^{\xi_2} d\xi\left[-\left|\tilde{E}_{ep}^{(n)}(S)\right|S + \left(\frac{1}{\xi} - \frac{2}{1+\xi^2}\right)\right]^{1/2} = \pi n\,, \tag{17}$$

where $\xi_{1,2}$ - the points of turn, the energy value $\left|\tilde{E}_{ep}^{(n)}(S)\right| = \left|E_{ep}^{(n)}(S)/E_{ep}^0\right|$. Leaving in the decomposition of the function under the integral symbol in (17) (with the parameter $\xi^2 \ll 1$) only the Coulomb part $(\sim \xi^{-1})$, one can receive the boundary transition of binding energy of parapositronium to its precise Coulomb spectrum

$$E_{ep}^{(n)} = -\frac{E_{ep}^0}{n^2} \tag{18}$$

in a nanopore of large radius *S*.

For a free radius *S* of a nanopore, the values of full energy $W_n(S)$ and also the binding energy $E_{ep}^{(n)}(S)$ of parapositronium, one can determine only numerously from the formulas (16) and (17) (the integrals in (16) and (17) can be expressed through tabulated elliptic integrals [10]). In Figs. 2 and 3 the dependencies $W_n(S)$ and $E_{ep}^{(n)}(S)$ on radius *S* of a nanopore are shown, which illustrate the numerous results obtained here.

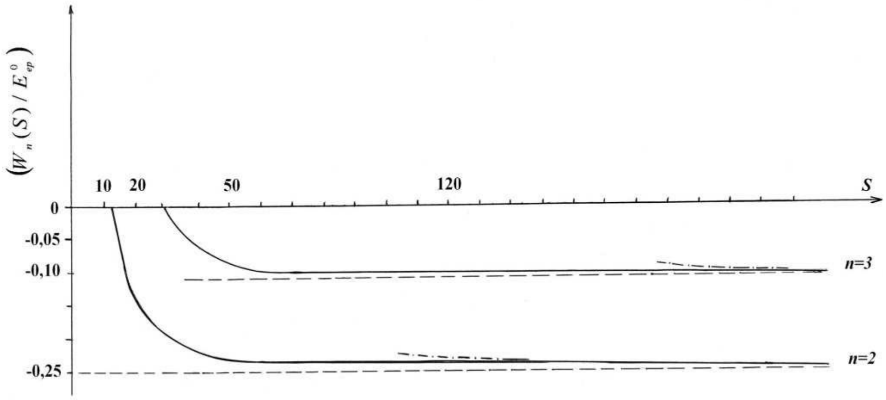

Fig. 2. The full energy $W_n(S)$ of electron-positron pare as a function of radius of a nanopore S (where $S = (a/a_{ep})$, a_{ep} - the Bohr radius of positronium in vacuum). The continuous lines - $W_n(S)$ in WKB approximation, the stroke-dotted lines - $W_n(S)$ (25) in the first order of the theory of perturbations. The value of binding energy of positronium $E_{ep}^0 = 1{,}70\,\text{eV}$ in dielectric medium located in a nanopore, represented by the dotted lines.

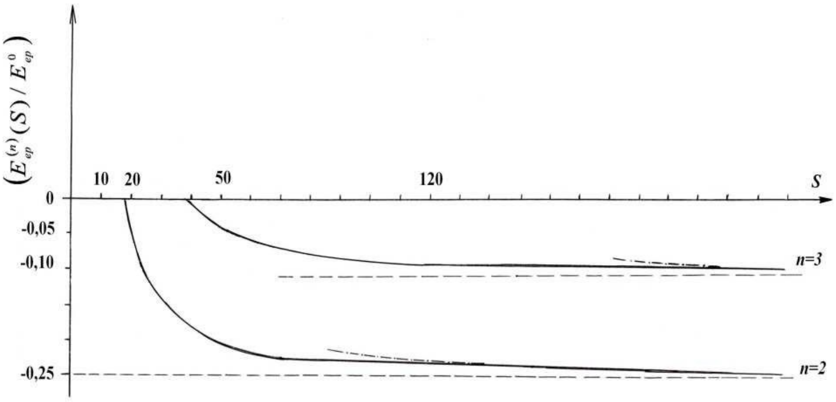

Fig. 3. The binding energy $E_{ep}^0(S)$ of electron-positron pare as a function of radius of a nanopore S (where $S = (a/a_{ep})$, the continuous lines - $E_{ep}^0(S)$ in WKB approximation, the stroke-dotted lines - $E_{ep}^0(S)$ (21) in the first order of the theory of perturbations. The value of binding energy of positronium $E_{ep}^0 = 1{,}70$ eV in dielectric medium located in a nanopore, represented by the dotted lines.

The dependence $E_{ep}(S)$ can be analysed for the only positronium states with their localization size being considerably less than radius S of nanopore. In this case, in the potential energy of gamiltonian $H(\rho, S)$ (14), the main part belongs to the values

$$\xi^2 = \left(\frac{\rho}{2a}\right)^2 \ll 1 \tag{19}$$

Therefore, leaving in the decomposition of potential energy the leading parts one can obtain the next expression for the gamiltonian of positronium $H(\rho, S)$ (14):

$$H(\rho, S) = -\frac{\hbar^2}{2\mu} \cdot \frac{1}{\rho} \cdot \frac{d}{d\rho}\left(\rho \frac{d}{d\rho}\right) - \frac{e^2}{\rho} + \frac{2}{S} E_{ep}^0 - \frac{2}{S} \xi^2 E_{ep}^0 \tag{20}$$

The main contribution to the binding energy of positronium is given by the energy of Coulomb interaction of electron with positron $V_{ep}(\rho)$ (7) (the second part in (20)). The two leaved parts in gamiltonian (20), describing the energy of interaction of electron and positron with the "strange" images (6), are taken into account in the first order of the theory of perturbations and give the addition to the Coulomb spectrum:

$$E_{ep}^{(n)}(S) = -\left[\frac{1}{n^2} - \frac{2}{S} + \frac{n^2(5n^2+1)}{4S^3}\right] E_{ep}^0 \qquad (21)$$

According to (19), as a criterion of applicability of existence of the positronium states studied here is the condition [11]:

$$\frac{n^2(5n^2+1)}{8S^2} \ll 1 \ , \qquad (22)$$

that together with demand of applicability of the first order of the theory of perturbations [11] reduces to such condition:

$$(2n^2/S) \ll 1 \ . \qquad (23)$$

Let us write down the gamiltonian of positronium in a nanopore of large radius S (23). Leaving in the decomposition of potential energy of gamiltonian $H(\rho, a)$(11) (with the parameter $\xi^2 \ll 1$) only the leading parts, one can receive the expression for the gamiltonian of positronium as follows:

$$H(\rho, S) = -\frac{\hbar^2}{2\mu} \cdot \frac{1}{\rho} \cdot \frac{d}{d\rho}\left(\rho \frac{d}{d\rho}\right) - \frac{e^2}{\rho} - \frac{4}{S}\xi^2 E_{ep}^0 \qquad (24)$$

In contrast to the gamiltonian of positronium (20), in that of (24) the dependence such as S^{-1} is absent, that is compensated by the contribution of energies of interaction of electron and positron with the "strange" (6) and their own (4), (5) images.

The decision of Shredinger equation (13) with gamiltonian (24) gives the spectrum of full energy of positronium moving in a nanopore of large radius S (23), as follows:

$$W_n(S) = -\left[\frac{1}{n^2} + \frac{n^2(5n^2+1)}{2S^3}\right] E_{ep}^0 \qquad (25)$$

The main contribution to the spectrum of full energy of positronium $W_n(S)$ (25) is given by the energy of Coulomb interaction of electron and positron (7) (the first part in (25)) and only as a correction is the second part in (25), caused by the energies of interaction of electron and positron with the "strange" (6) and their own (4), (5) images. The expression (25) was obtained with the use of the first order of the theory of perturbations. In making so the condition of applicability of the first order of the theory of perturbations reduces to the inequality (23).

The expressions found describing the full energy spectrum of positronium $W_n(S)$ (25) and the binding energy of positronium $E_{ep}^{(n)}(S)$ (21), are applicable only for the lowest positronium states *(n)*, for that the inequality is valid

$$\left|E_{ep}^{(n)}(S)\right|, \ |W_n(S)| \ll \Delta V \ , \qquad (26)$$

where $\Delta V \approx 4{,}5 \ eV$ - the energy of electronic relation at the "nanopore-matrix" interface [12]. It should be noted that the full energy of positronium $W_n(S)$ (25) in a nanopore of radius S is counted off from the vacuum standard.

The absorption spectra of light by the positronium states in the nanopores of solid matrices:-

Let us carry out the qualitative valuation of the quantities of binding energy $E_{ep}^{(n)}(S)$ and full energy $W_n(S)$ of parapositronium moving in a nanopore (with permittivity $\varepsilon_2 = 2$) of radius *S* (2a) in solid matrices (with permittivity $\varepsilon_1 = 4$). The fulfillment of conditions (2*a*), (23), (26) results in that to exist in the bulk of nanopore only the finite number of parapositronium states (*n*), starting with the states $n \geq 2$. To simplify, without decreasing generality, let us study here only the positronium states *n* = 2 и 3. The theory developed by us (the conditions (2a), (23), (26)) are fulfilled) gives a possibility to analyze the positronium states (*n* = 2 и *n* = 3) in nanopores, starting with radiuses $a \geq$ 2 nm (2a).

The full energy of positronium $|W_n(a)|$, obtained with the help of WKB method in a nanopore of radius *a* (2a), and also in the framework of the first order of the theory of perturbations (25) in a nanopore of large radius *a* (23), with growing radius *a* for positronium states (*n* = 2 и *n* = 3) is increasing (Fig. 2). In making so, the values of full energy of positronium $W_n(a)$ (25) in a nanopore, starting with radius of 11 nm (or $S \geq 104$) (for the states with *n* = 2) , and also in a nanopore, starting with radius $a \geq 20{,}4$ nm (or $S \geq 192$) (for the states with *n* = 3), are slightly different (within the limits do not exceeding 10%) from the full energy value obtained by WKB method (Fig. 2). Starting with the radiuses of nanopores $\bar{a}_2 \approx 555$ nm (or $\bar{S}_2 \approx 524$) (for the state with *n* = 2) and $\bar{a}_3 \approx 763$ nm (or $\bar{S}_3 \approx 720$) (for the state with *n* = 3), the full energy of parapositronium asymptotically tends to the values (15), characterizing the positronium states in vacuum (Fig. 2). The values of full energy of parapositronium $W_n(a)$ refer to the infrared (the states with *n* = 2 and *n* = 3) spectrum area.

From Fig. 3 showing the dependence of binding energy of parapositronium $E_{ep}^{(n)}(S)$ on radius *a* of a nanopore which has been obtained by WKB method, it follows that the bound states of electron-positron pare arise in a nanopore, starting with the value of radius $a \geq a_c^{(2)} \approx 1{,}81$ *nm* (or $S \geq S_c^{(2)} \approx 17{,}1$) (for the states with *n* = 2) and for the states with *n* = 3 in a nanopore, starting with the value of radius $a \geq a_c^{(3)} \approx 4{,}1$ *nm* (or $S \geq S_c^{(3)} \approx 38{,}2$). In making so, the states of electron-positron pare, starting with a nanopore of radius $a \geq a_c^{(2)}$ (for the states with *n* = 2), and starting with a nanopore of radius $a \geq a_c^{(3)}$ (for the states with *n* = 3), are found in the area of negative energies with this corresponding to the bound state of electron and positron. In this case, the energy of Coulomb interaction $V_{ep}(\rho)$ (7) between electron and positron, and also the energy of polarization interaction $U(\rho, a)$ (3)-(6) of electron and positron with a spherical "nanopore-matrix" interface, exceed the energy of dimensional quantation of electron and positron in a nanopore.

The binding energy of positronium $E_{ep}^{(n)}(a)$ (21) in a nanopore of large radius *a* (23), obtained with the help of the first order of the theory of disturbances, starting with a nanopore of radius $a \geq 8{,}9$ nm (or $S \geq 84$) (for the states with *n* = 2), and starting with a nanopore of radius $a \geq 19{,}1$ nm (or $S \geq 180$) (for the states with *n* = 3), acquires the values that are slightly different (within the limits do not exceeding 11%) from the binding energy obtained by WKB method (Fig. 3). With growing radius *a* of a nanopore the increase in the binding energy $\left|E_{ep}^{(n)}(a)\right|$ of parapositronium is observed (Fig. 3). Starting with the values of nanopore radiuses $\tilde{a}_2 \approx 50{,}9$ nm (or $\tilde{S}_2 \approx 480$) (for the states with *n* = 2) and $\tilde{a}_3 \approx 73{,}1$ nm (or $\tilde{S}_3 \approx 690$) (for the states with *n* = 3), the binding energy of parapositronium asymptotically tends to the values (18), characterizing the positronium states in a nanopore (with permittivity $\varepsilon_2 = 2$) (Fig. 3). The values of binding energy $E_{ep}^{(n)}(a)$ of parapositronium are arranged in the infrared (*n* = 2 and *n* = 3) area of spectrum.

As a bulk positronium in a nanopore one can understand positronium with its parameters (the reducted effective mass, the Bohr radius, the binding energy) in a nanopore do not differing from these in a medium with permittivity $\varepsilon_2 = 2$. A bulk parapositronium appears in the state with *n* = 2 only in a nanopore, starting with radius $a \geq \tilde{a}_2 \approx 50{,}9$ nm and in the state with *n* = 3 only in a nanopore, starting with radius $a \geq \tilde{a}_3 \approx 73{,}1$ nm (Figs. 2 and 3).

For positronium states with *n* = 2 and *n* = 3 to exist in a nanopore of radius *a* at the temperatures $T \ll T_1$, there is necessity for the condition

$$k_B T \ll k_B T_1 \equiv \left|E_{ep}^{(n)}(a)\right|, \qquad (27)$$

to be fulfilled (where k_B – the Boltzmann constant), which is satisfied up to the temperatures of melting the matrix.

The investigations of parapositronium states with *n* = 2 and *n* = 3 in nanopores of radiuses *a* (2a), (18), (23), located in the pores of solid matrices, are possible in the processes of absorption (radiation, reflection) in the transitions with frequencies

$$\hbar\omega_n^{n'}(a) = \Delta W_n^{n'}(a) = \left| W_{n'}(a) - W_n(a)\right|, \qquad (28)$$

arranged in the infrared spectrum area (Table). In formula (28) the values of full energy $W_n(a)$ (where *n* = 2 и *n′* = 3) were obtained by WKB method (Fig. 2). In nanopores with radiuses $a \geq a_c^{(3)}$, absorption (radiation, reflection) is contributed by the states with *n* = 2 and *n* = 3. Therefore, one can spectroscopically control the rise of nanopores (i.e. the origination of new phase), starting with sizes $a \geq a_c^{(3)} \approx 4{,}1$ nm in solid matrices. With growing radius *a* of a nanopore from $a = 4{,}5$ nm ($S = 42{,}5$) to $a = 11{,}0$ nm ($S = 103{,}8$), the frequencies of transitions (28) between parapositronium states with *n* = 3 and *n* = 2 are monotonously diminishing from 0,273 eV to 0,235 eV (Table).

The energy interval between the parapositronium levels participating in the processes of absorption (radiation, reflection) would be an order of several $k_B T$. In making so, the inequality

$$k_B T \ll k_B T_2 \equiv \Delta W_n^{n'}(a), \qquad (29)$$

would be fulfilled, where the values of full energy $W_n(a)$ (*n* = 2 and *n′* = 3) was obtained by WKB method (Fig. 3). In making so, the condition (29) is fulfilled up to the temperatures of melting the matrix.

Table

The frequencies of transitions $\hbar\omega_n^{n'}(a)$ (28) between the energy levels (*n'* = 3 and *n* = 2) as functions of radius of a nanopore *a*. The frequencies of transitions $\hbar\omega_n^{n'}(a)$, expressed in units E_{ep}^{0}

(8) (and also in eV); radiuses of nanopores *a* expressed in nm (and also innondimensional units $S = \left(a/a_{ep}\right)$ (where a_{ep} - the Bohr radius of positronium in vacuum)).

a, nm *(S)*	$\frac{\left(W_3(a) - W_2(a)\right)}{E^0_{ep}}$ (eV)
4,5 (21,3)	0,16 (0,273)
5,0 (23,6)	0,15 (0,255)
6,0 (28,3)	0,146 (0,25)
7,0 (33)	0,143 (0,244)
8,0 (37,8)	0,142 (0,0242)
9,0 (42,5)	0,141 (0,24)
10,0 (47,2)	0,14 (0,238)
11,0 (52,0)	0,139 (0,235)

CONCLUSION

The peculiarities of parapositronium states discovered connected with the dependence of their binding energy $E_{sp}^{(n)}(a)$ and full energy $W_n(a)$ on sizes a of nanopores can be interesting for development of the new method for optical control of porous structure of materials. The new method for determination of sizes a of nanopores is based on comparison of the experimental spectra of absorption (radiation, reflection) of positronium in nanopores with theoretical dependencies of energy spectra of positronium (16), (25), (28) on radius a of nanopores. With the help of the method proposed one can determine the values of radiuses of nanopores $a_c^{(2)}$ (for the states with $n = 2$) and $a_c^{(3)}$ (for the states with $n = 3$), starting with which in nanopores of size $a \geq a_c^{(2)}$ and $a \geq a_c^{(3)}$ the bound states of electron-positron pare arise, and also appreciate the concentration of pores n (the value being an order of a^{-3}), and consequently to appreciate the porosity (degree of dispersion) of matrix. The development of such optical method can be of separate interest to control the rise of defects or the origins of new phase (for example, nanopores) on radiation or heat impacts onto multicomponent nanostructures [1-4, 7,8], and also the influence of extreme conditions onto the properties of materials (the explosive synthesis of crystals, hydrobreak of a layer and so on).

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