PHYSICS AND CHEMISTRY OF SOLID STATE
V. 24, No. 1 (2023) pp. 146-152

Section: Physics

DOI: 10.15330/pcss.24.1.146-152

Vasyl Stefanyk Precarpathian National University

ФІЗИКА І ХІМІЯ ТВЕРДОГО ТІЛА
Т. 24, № 1 (2023) С. 146-152

Фізико-математичні науки

PACS: 71.20.-b

ISSN 1729-4428

I.V. Bilynskyi, R.Ya. Leshko, H.Ya. Bandura

Electron and hole spectrum taking into account deformation and polarization in the quantum dot heterostructure InAs/GaAs

Physics Department, Drohobych Ivan Franko State Pedagogical University, Drohobych, Ukraine, galinka.bandura@gmail.com

In the paper InAs spherical quantum dots in a GaAs matrix were investigated. The energies of electrons and holes in single- and multi-band models (with strong, weak, and intermediate spin-orbit interaction) were calculated taking into account both the deformation of the quantum-dot matrix and the polarization charges on the quantum dot surface. The dependence of the energy levels of electrons and holes on the radius of the quantum dot is considered. It is shown that the deformation effects are stronger than polarization for the electron. For holes those effects are opposites. The energies of electrons and holes have been compared in all approximation models.

Keywords: exchange interaction, deformation, 4-band model or multiband hole model, 6-band model, polarization charges, strained heterosystem.

Received 31 October 2022; Accepted 21 February 2023.

Introduction

Recently much attention has been paid to the physics of low-dimensional semiconductor structures. This has been stimulated by the rapid progress in nanometer-scale fabrication technology. Among them, quantum dots, which are also defined as nanocrystals and microcrystallites, or nanoclusters, are of particular interest. The effect of quantum confinement on electrons and holes in semiconductor quantum dots (QD) has been studied in [1-3].

The superlattices of quantum dots InAs in a matrix GaAs has been studied in [4]. The superlattices of spherical and cubic quantum dots (QD) have been studied. Using the method of plane waves for different shapes of QD, analytical expressions for calculating the energy spectrum have been obtained. The dependences of energy zones at high symmetry dots have been constructed. Dependences of the the widths of zones have been found.

The basis for the creation of optoelectronic devices is a single-particle character - an electron and a hole. Analytical expressions describing the energy spectrum of electrons and holes for a quantum dot (QD) arising in a self-consistent deformation field created by an array of coherently stressed QDs were obtained in the paper [5]. It is shown that the internal elastic deformation that occurs at the boundary of the QD matrix affects the energy spectrum of electrons more significantly than the spectrum of holes. The interaction of quantum dots (QDs) between themselves and external electromagnetic fields depends on the size and geometry of quantum dots [6-9]. These dependencies are used in various electronic and optoelectronic devices, including lasers [10-12], single-photon sources [13-15], solar cells [16-18], and photodetectors [19, 20].

Theoretical models for three-dimensional superlattices of cubic and tetragonal InAs/GaAs and Ge/Si quantum dots are proposed in works [21, 22]. Electronic and phonon spectra of such superlattices, densities of electronic states, the effective mass tensor, and conductivity were studied. It was established that the properties of three-dimensional superlattices of quantum dots are more sensitive to the distance between dots than to the shape of the dots.

Real structures can contain various defects. Therefore, conditions may change. For heterosystems in which there is a large difference between the dielectric constants, the effect of polarization charges will be significant. The change in the dielectric properties of the matrix taking into account the polarization or deformation charges leads to a significant change in the energy of both the electron and the hole. It should be reflected in the optical and other QD properties.

In view of this, in our work we have been calculated the energies of the electron in singleband model, and the hole in both singleband and multiband-band model approximation. And we also have been calculated electron and hole energies with the deformation and polarization at the same time.

I. Electron energies of semiconductor quantum dots

Let's write the Hamiltonian of the electron in the form

$$\hat{H}_e = -\frac{1}{2}\nabla\frac{1}{m_e}\nabla + U(r_e) = \frac{1}{2}\nabla\frac{1}{m_e}\nabla + U_{conf}(r_e) + U_d(r_e) + U_p(r_e) = \hat{H}_e^0 + U_d(r_e) + U_p(r_e) \quad (1)$$

where

$$m_e = \begin{cases} m_e^{(1)}, & r_e \le \alpha, \\ m_e^{(2)}, & r_e > \alpha. \end{cases}$$

$$U_{conf}\left(r_{\{e \atop r\}}\right) = \begin{cases} 0, & r_{\{e \atop r\}} \le \alpha, \\ U_{0;\{e \atop r\}} & r_{\{e \atop r\}} > \alpha. \end{cases} \quad (2)$$

$$U_d\left(r_{\{e \atop h\}}\right) = \begin{cases} 0, & r_{\{e \atop h\}} \le \alpha, \\ U_{0,d;\{e \atop h\}} & r_{\{e \atop h\}} > \alpha, \end{cases} = \begin{cases} 0, & r_{\{e \atop h\}} \le \alpha, \\ -\left|D^{(1)}_{\{e \atop h\}}\varepsilon^{(1)}\right| - \left|D^{(2)}_{\{e \atop h\}}\varepsilon^{(2)}\right| & r_{\{e \atop h\}} > \alpha, \end{cases} \quad (3)$$

$$U_p\left(r_{\{e \atop h\}}\right) = \frac{\gamma_0}{4\chi\left(r_{\{e \atop h\}}\right)}\int_0^\infty d\,r_0 \frac{th\left(\frac{r_0-\alpha}{L}\right) + \frac{r_0}{L}sech^2\left(\frac{r_0-\alpha}{L}\right)}{r_0^2 - r_{\{e \atop h\}}} \quad (4)$$

When $U_d(r) = 0$, $U_p(r) = 0$, polarization and deformation can be neglected. The Schrödinger equation with and without account the QD deformation can be solved exactly. It has an expression for the ground state

$$\psi_{e;m_s}(\vec{r}_e) = \frac{1}{\sqrt{4\pi}}S_{e;m_s}\begin{cases} A_e^{(1)}\frac{J_{1/2}(kr_e)}{\sqrt{r_e}}, & r_e \le \alpha, \\ A_e^{(2)}\frac{K_{1/2}(\eta r_e)}{\sqrt{r_e}}, & r_e > \alpha, \end{cases} = \frac{1}{\sqrt{4\pi}}S_{e;m_s}\begin{cases} A_e^{(1)}\frac{sin(kr_e)}{r_e}, & r_e \le \alpha, \\ A_e^{(2)}\frac{exp(-\eta r_e)}{r_e}, & r_e > \alpha, \end{cases} \quad (5)$$

where $S_{e;m_s}$ is spin function, $m_s = \pm\frac{1}{2}$, $k = \sqrt{2m_e^{(1)}E}$. $\eta = \sqrt{2m_e^{(2)}(U_{0;e} - E)}$ when the QD deformation is neglected and $\eta = \sqrt{2m_e^{(2)}(U_{0;e} + U_{0,d;e} - E)}$ when the QD deformation is accounted. Taking into account the boundary condition and normalize condition, the wave functions and electron energies have been defined. The influence of polarization charges has been calculated in the first-order of perturbation theory. In the same manner the hole energies have been obtained in the case when one can neglect the complex band structure (only heavy hole band is accounted).

In real situation for the InAs/GaAs heterosystem the multiband model for hole states should be used. In the multiband model approximation in the case of intermediate spin-orbit interaction (so-called 6-band model), the solutions of the Schrödinger equation with the Hamiltonian [23-25] have the form like in [23]:

$$\psi_j^+ = \begin{pmatrix} \frac{R_{h2}^+}{\sqrt{2j(2j-1)(2j-2)}}\Phi_{j-3/2}^{(4)} + \frac{R_{h1}^+}{\sqrt{2j(2j+2)(2j+3)}}\Phi_{j+1/2}^{(4)} \\ R_S^+\Phi_{j+1/2}^{(2)} \end{pmatrix},$$

$$(6)$$

$$\psi_j^- = \begin{pmatrix} \frac{R_{h2}^-}{\sqrt{2(j+1)(2j+3)(2j+4)}}\Phi_{j+3/2}^{(4)} + \frac{R_{h1}^+}{\sqrt{2j(2j-1)(2j+2)}}\Phi_{j-1/2}^{(4)} \\ R_S^-\Phi_{j-1/2}^{(2)} \end{pmatrix},$$

where $\Phi_k^{(4)}$, $\Phi_k^{(2)}$ are four-dimensional and two-dimensional vectors-columns [24] based on spherical harmonics $Y_{l,m}(\theta,\varphi)$. We obtain two systems of equations for the radial components of the holes eigenfunctions, R_{h1}, R_{h2}, R_S are located in the QD and outside QD $\left(j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}\dots\right)$..

Systems of differential equations have exact solutions for even and odd states. In the inner region for a spherical QD, the solutions of the equations system (radial functions), are written using the sum of the three spherical Bessel functions of the first kind:

$$
\begin{gathered}
R_{h1}^{j+}(r) = C_1 J_{j+1/2}(k_l r) + c_2 J_{j+1/2}(k_h r) + C_3 J_{j+1/2}(k_s r), \\
R_{h2}^{j+}(r) = -C_1\sqrt{\frac{3(2j-1)}{2j+3}} J_{j-3/2}(k_l r) + C_2\sqrt{\frac{3(2j+3)}{3(2j-1)}} J_{j-3/2}(k_h r) - C_3\sqrt{\frac{3(2j-1)}{2j+3}} J_{j+3/2}(k_s r), \\
R_s^{j+}(r) = -C_1\sqrt{\frac{j}{2j+3}}\frac{2E-(\gamma_1+2\gamma)k_l^2}{\gamma k_l^2} J_{j+\frac{1}{2}}(k_l r) + C_3\sqrt{\frac{j}{2j+3}}\frac{2E-(\gamma_1+2\gamma)k_s^2}{\gamma k_s^2} J_{j+\frac{1}{2}}(k_s r),
\end{gathered} \tag{7}
$$

and solutions for odd states

$$
\begin{gathered}
R_{h1}^{j-}(r) = C_4\sqrt{2j-1} J_{j-1/2}(k_l r) + c_5\sqrt{2j-1} J_{j-1/2}(k_h r) + c_6\sqrt{2j-1} J_{j-1/2}(k_s r), \\
R_{h2}^{j-}(r) = C_4\sqrt{3(2j+3)} J_{j+3/2}(k_l r) + C_5\sqrt{\frac{2j-1}{3(2j+3)}} J_{j+3/2}(k_h r) + C_6\sqrt{3(2j+3)} J_{j+3/2}(k_s r), \\
R_s^{j-}(r) = C_4\sqrt{j+1}\frac{(\gamma_1+2\gamma)k_l^2-2E}{\gamma k_l^2} J_{j-1/2}(k_l r) + C_6\sqrt{j+1}\frac{(\gamma_1+2\gamma)k_s^2-2E}{\gamma k_s^2} J_{j-1/2}(k_s r),
\end{gathered} \tag{8}
$$

where

$$
\begin{gathered}
k_h^2 = \frac{2E}{\gamma_1-2\gamma}, \\
k_{l,s}^2 = \frac{2E(\gamma_1+\gamma)-\Delta(\gamma_1+2\gamma)\pm\sqrt{[2E(\gamma_1+\gamma)-\Delta(\gamma_1+2\gamma)]^2-4E(E-\Delta)(\gamma_1-2\gamma)(\gamma_1+4\gamma)}}{(\gamma_1-2\gamma)(\gamma_1+4\gamma)}.
\end{gathered} \tag{9}
$$

Δ is the value of spin-orbit interaction. In the matrix ($r>a$), the solutions of the equations can be represented using modified Bessel functions of the second kind for even and odd states:

$$
\begin{gathered}
R_{h1}^{j+}(r) = c_1 K_{j+1/2}(k_l r) + c_2 K_{j+1/2}(k_h r) + c_3 K_{j+1/2}(k_s r), \\
R_{h2}^{j+}(r) = -c_1\sqrt{\frac{3(2j-1)}{2j+3}} K_{j-3/2}(k_l r) + c_2\sqrt{\frac{2j+3}{3(2j-1)}} K_{j-3/2}(k_h r) - c_3\sqrt{\frac{3(2j-1)}{2j+3)}} K_{j+3/2}(k_s r), \\
R_s^{j+}(r) = c_1\sqrt{\frac{j}{2j+3}}\frac{2\varepsilon-(\gamma_1+2\gamma)k_l^2}{\gamma k_l^2} K_{j+1/2}(k_l r) + c_3\sqrt{\frac{j}{2j+3}}\frac{2\varepsilon-(\gamma_1+2\gamma)k_s^2}{\gamma k_s^2} K_{j+1/2}(k_s r),
\end{gathered} \tag{10}
$$

$$
\begin{gathered}
R_{h1}^{j-} = c_4\sqrt{2j-1}\, K_{j-1/2}(k_l r) + c_5\sqrt{2j-1}\, K_{j-1/2}(k_h r) + c_6\sqrt{2j-1}\, K_{j-1/2}(k_s r), \\
R_{h2}^{j-} = c_4\sqrt{3(2j+3)}\, K_{j+3/2}(k_l r) - c_5\frac{\sqrt{2j-1}}{\sqrt{3(2j+3)}} K_{j+3/2}(k_h r) + c_6\sqrt{3(2j+3)}\, K_{j+3/2}(k_s r), \\
R_s^{j-}(r) = c_4\sqrt{j+1}\,\frac{(\gamma_1+2\gamma)k_l^2-2E}{\gamma k_l^2} K_{j-1/2}(k_l r) + c_6\sqrt{j+1}\,\frac{(\gamma_1+2\gamma)k_s^2-2E}{\gamma k_s^2} K_{j-1/2}(k_s r),
\end{gathered} \tag{11}
$$

The squares of wave vectors k_l, k_h, k_s are obtained from the formula (9) by substitution $E \to E - U_{0,h}\gamma_1 \to \gamma_1^{II}$, $\gamma \to \gamma^{II}, \Delta \to \Delta^{II}.\gamma, \gamma_1$ - are the Luttinger parameters which set the effective masses of heavy and light holes:

$$
m_l = m_0/(\gamma_1+2\gamma),\ m_h = m_0/(\gamma_1-2\gamma),
$$

$$
\begin{cases}\gamma_1, & r \le \alpha, \\ \gamma_1^{II}, & r > \alpha,\end{cases} \qquad \begin{cases}\gamma, & r \le \alpha, \\ \gamma^{II}, & r > \alpha.\end{cases}
$$

m_0 - is free-electron mass.

If in formulas (7) - (11) the value of Δ is very large, then we obtain the results, which describe multiband hole model in the case of strong spin-orbit interaction (so-called 4-band model) which doesn't take into account the spin-orbital band. If we assume that $m_l = m_h$ and Δ is very large, then we get single band model.

To account the deformation in (7)-(11), the substitution $U_{0,h} \to U_{o,h} + U_{o,d;h}$ should be done. When we use the boundary condition [23] and normalize condition the hole energy spectrum can be calculated with take into account the QD-matrix deformation. Polarization charges can be accounted in the perturbation theory.

II. Results

Specific calculations have been performed for heterosystem InAs/GaAs. The parameters are given in table 1. We have proposed the model which accounts for the polarization charges at the QD surface and deformation of the QD and matrix.

Table 1.

The effective masses

	$m^{(1)}$	$m^{(2)}$	U_0
Electron	0.023	0.067	0.83
heavy hole	0.41	0.51	0.262
light hole	0.026	0.082	0.33

In fig. 1 shows the dependence of the electron energy on the QD radius without polarization and deformation (curve 1), with polarization (curve 2), with deformation (curve 3), with both polarization and deformation (curve 4). We see that for an electron, the energy with only polarization is the highest, and only with deformation is the lowest in compare without them. If we consider the energy with both polarization and deformation, it can be seen that the effects of deformation are stronger for the electron than the effects of polarization. This can be explained as follows: large constants of the hydrostatic deformation potential for electrons and a small difference between the values of the dielectric constant of the QD and the matrix.

In fig. 2 shows the dependence of the heavy hole energy on the radius without polarization and deformation (curve 1), with polarization (curve 2), with deformation (curve 3), and also with polarization and deformation (curve 4). We can see that for the hole the energy plot with only polarization is the highest. And only with deformation is the lowest. But for a hole, the deformation effects are weaker than the polarization effects. The reason for this is the smaller values of the constants of the hydrostatic deformation potential of the holes. And in total energy are lager (curve 4 is higher than curve 1).

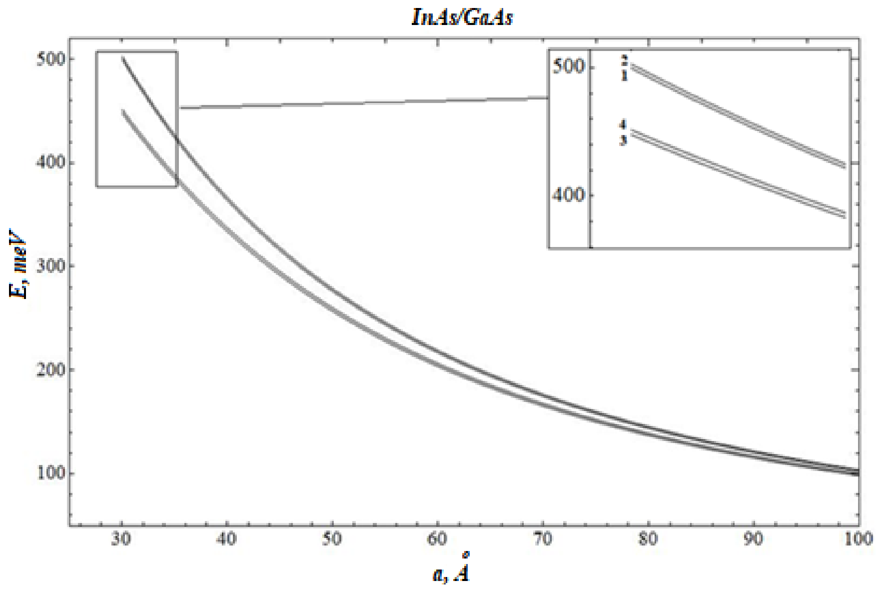

Fig.1. Dependence of the electron ground state energy on the radius of the QD:
1 – without taking into account polarization and deformation effects; 2 – with account only polarization charges; 3 – with account only deformation; 4 – with account both polarization and deformation.

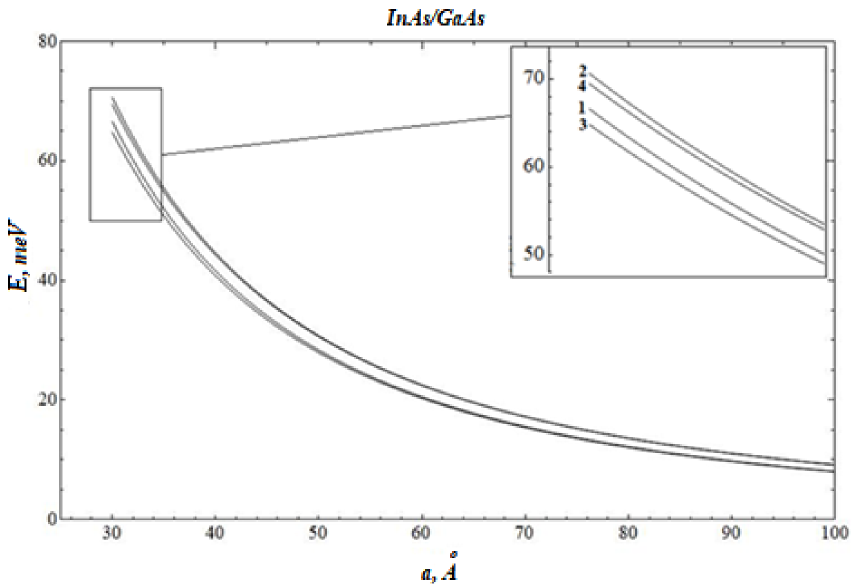

Fig.2. Dependence of the heavy hole ground state energy on the radius of the quantum dot:
1 – without taking into account polarization and deformation effects; 2 – with account only polarization charges; 3 – with account only deformation; 4 – with account both polarization and deformation.

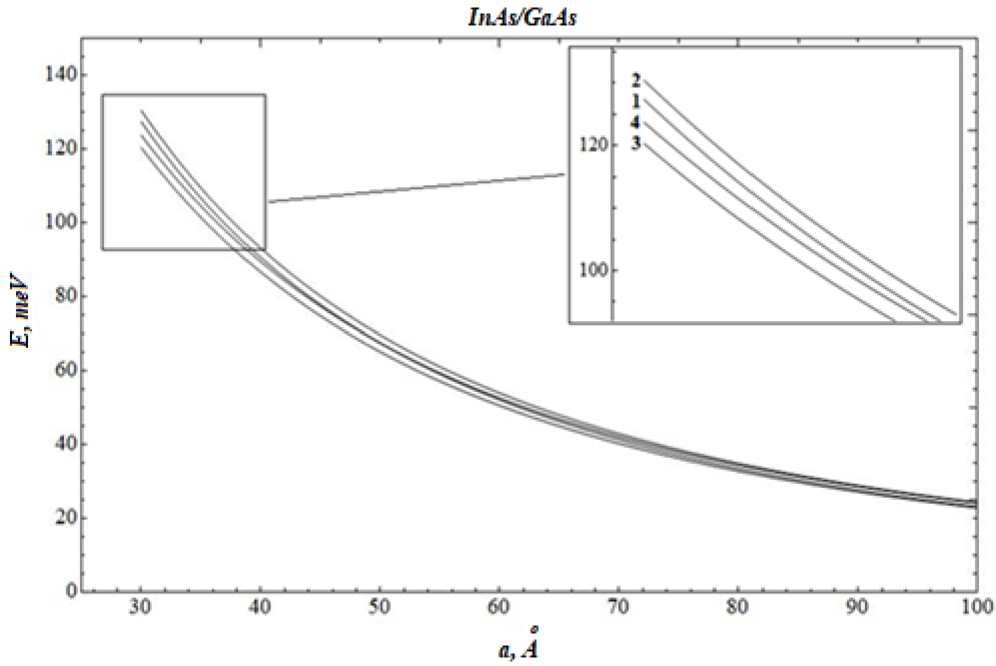

Fig.3. Dependences of ground state hole energies on the QD radius in the 4-band model approximation: 1 – without taking into account polarization and deformation effects; 2 – with account only polarization charges; 3 – with account only deformation; 4 – with account both polarization and deformation.

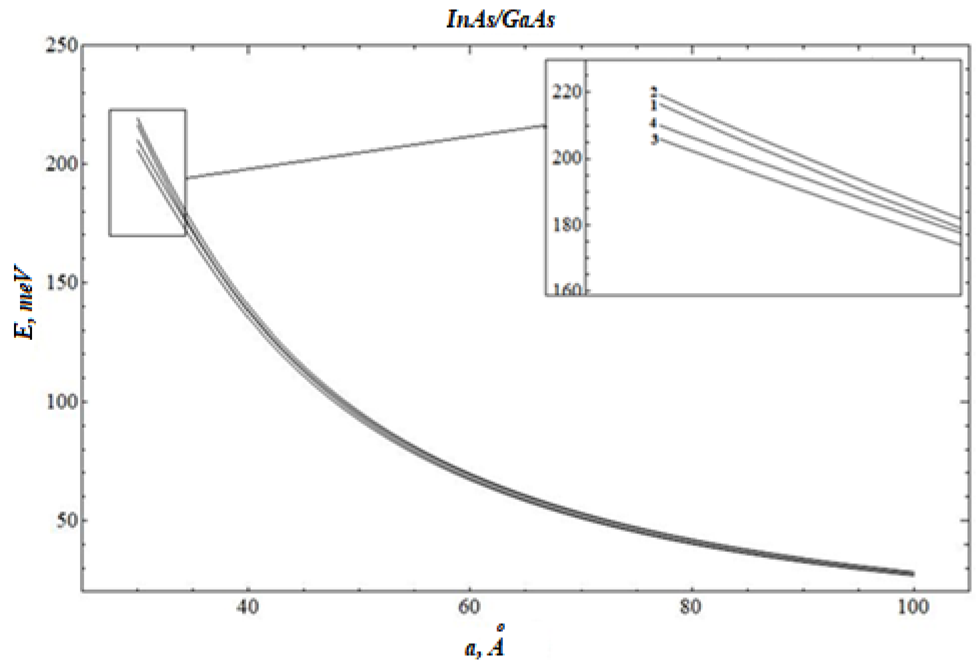

Fig.4. Dependences of ground state hole energies on the QD radius in the 6-band approximation: 1 – without taking into account polarization and deformation effects; 2 – with account only polarization charges; 3 – with account only deformation; 4 – with account both polarization and deformation.

Fig. 3 and fig. 4 show the dependences of the energies on the radius in the 4-band and 6-band approximation. The effects of deformation and polarization are similar to those of an electron, but they are different in magnitude. That is why we compare energies in all presented model for hole (fig. 5). It shows the dependence of the hole energy of various QD radius, taking into account both polarization and deformation. Curve 1 is responsible for the electron, curves 2 and 5 are energies of the light and heavy hole, curve 3 and 4 describe the hole energy in the 4-band and 6-band models, respectively. We can see that the energy for the hole is lower than that for the electron. It caused by effective masses, which for the electron is larger. Also, we have been noted, that in the case of the model with intermediate spin-orbit interaction (6-band model) the energies are larger than in the 4-band model (with large spin-orbit interaction, when spin-off band are neglected). Those result obtained when polarization and deformation are accounted. If polarization and deformation are neglected, the hole energy in the 6-band model are smaller

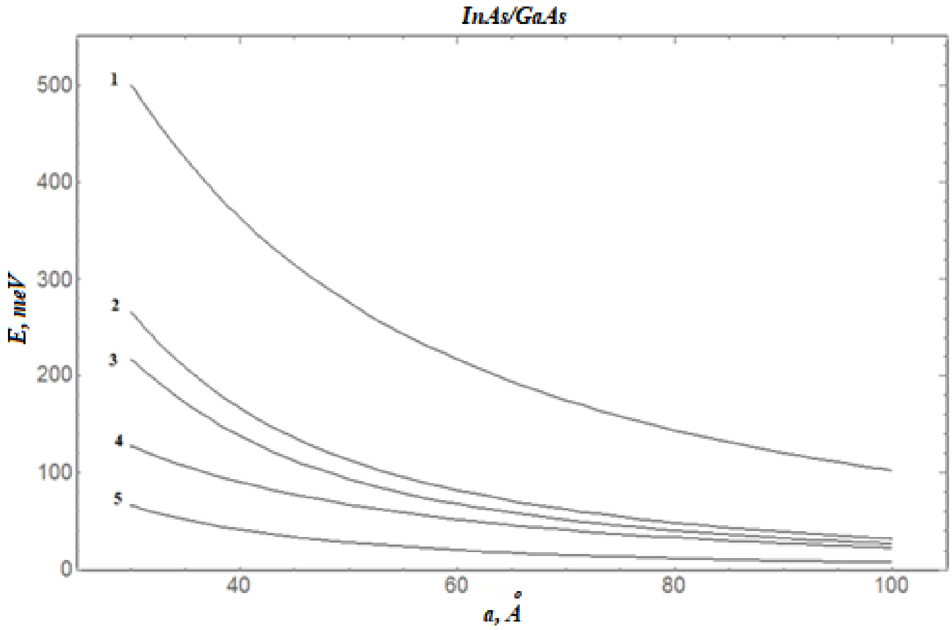

Fig.5. Dependence of ground state energy on QD radius for: 1 – for electron; 2 – singleband model for light hole; 3 - 6-band approximation model for hole; 4 – 4-band approximation model for hole; 5 – singleband model for heavy hole.

than 4-band [23]. Those results for hole are caused by the larger influence of the polarization in the 6-band model than deformation.

Conclusions

In this paper for InAs/GaAs heterosystem we perform calculation of electron and hole energies in single and multiband models with account both QD-matrix deformation and polarization charges on the surface. For electron the deformation effects are stronger. Form holes the polarization are stronger. If we compare hole models, the deformation and polarization are partially compensated, but in the total effect the polarization is stronger (curves 4 are higher than 2 in fig.2-3) in all models. Also, in the 6-band model total hole energies (with account polarization and deformation) are larger than in the case of 4-band model for all QD radiuses, especially for small QD radiuses the difference is signified. For large QD radiuses the difference is vanished.

Bilynskyi I.V. – Doctor of Physical and Mathematical Sciences, Professor of Physics Department;
Leshko R.Ya. – Candidate of Physical and Mathematical Sciences, docent of Physics Department;
Bandura H.Ya. – PhD student of Drohobych Ivan Franko State Pedagogical University.

[1] J.B. Xia and J.B. Li, *Electronic structure of quantum spheres with wurtzite structure*, Phys. Rev. B, 60, 11 540 (1999); https://doi.org/10.1103/PhysRevB.60.11540.

[2] A. Lochmann, E. Stock, O. Schulz, F. Hopfer, D. Bimberg, V. Haisler, A. Toporov, A. Bakarov, and A. Kalagin, *Electrically driven single quantum dot polarised single photon emitter*, Electron. Lett., 42, 774 (2006); https://doi.org/10.1049/el:20061076.

[3] M. Scholz *et al.*, Non-classical light emission from a single electrically driven quantum dot, Opt. Express, 15, 9107 (2007); https://doi.org/10.1364/OE.15.009107.

[4] I. Bilynskyi, R. Leshko, & H.Bandura, *Influence of quantum dot shape on energy spectra of three-dimensional quantum dots superlattices*, Physics and Chemistry of Solid State, 21(4), 584 (2020); https://doi.org/10.15330/pcss.21.4.584-590.

[5] O. O. Dan'kiv, R. M. Peleshchak, *Strain-renormalized energy spectra of electrons and holes in InAs quantum dots in the InAs/GaAs heterosystem*, Technical Physics Letters, 31, 691 (2005);

[6] I. D. Rukhlenko et al., *Kinetics of pulse-induced photoluminescence from a semiconductor quantum dot*, Opt. Express 20, 27612 (2012); https://doi.org/10.1364/OE.20.027612.

[7] A.S. Baimuratov, V.K. Turkov, I.D. Rukhlenko, A.V. Fedorov, *Shape-induced anisotropy of intraband luminescence from a semiconductor nanocrystal*, Opt. Lett., 37, 4645 (2012); https://doi.org/10.1364/OL.37.004645.

[8] D. Press, T.D. Ladd, , D. P. Y. Yamamotol, B. Zhang, *Complete quantum control of a single quantum dot spin using ultrafast optical pulses*, Nature, 456, 218 (2008); https://doi.org/10.1038/nature07530.

[9] A.V. Baranov, A.V. Fedorov, I.D. Rukhlenko, Y. Masumoto, *Intraband carrier relaxation in quantum dots embedded in doped heterostructures,* Phys. Rev. B, 68, 205318 (2003); https://doi.org/10.1103/PhysRevB.68.205318.
[10] A.J. Shields, *Semiconductor quantum light sources*, Nat. Photon., 1, 215 (2007); https://doi.org/10.1038/nphoton.2007.46.
[11] K.J. Vahala, *Optical microcavities*, Nature, 424, 839 (2003); https://doi.org/10.1038/nature01939.
[12] V.I. Klimov, A.A. Mikhailovsky, S. Xu, A. Malko, *Optical gain and stimulated emission in nanocrystal quantum dots*, Science, 290, 314 (2000); https://doi.org/10.1126/science.290.5490.314.
[13] Z.L. Yuan et al., *Electrically Driven Single-Photon Source*, Science, 295, 102 (2002); https://doi.org/10.1126/science.1066790.
[14] A.J. Bennett et al., *Microcavity single-photon-emitting diode*, Appl. Phys. Lett., 86, 181102 (2005); https://doi.org/10.1063/1.1921332.
[15] P. Michler et al., *A Quantum Dot Single-Photon Turnstile Device*, Science, 290, 2282 (2000); https://doi.org/10.1126/science.290.5500.2282.
[16] K. Tanabe, K. Watanabe, Y. Arakawa, *III-V/Si hybrid photonic devices by direct fusion bonding*, Scientific Rep., 2, 349 (2012); https://doi.org/10.1038/srep00349.
[17] J. Jasieniak, B.I. MacDonald, S. E. Watkins, P. Mulvaney, *Solution-processed sintered nanocrystal solar cells via layer-by-layer assembly*, Nano Lett., 11(7), 2856 (2011); https://doi.org/10.1021/nl201282v.
[18] I. Gur, N.A. Fromer, M.L. Geier, A.P. Alivisatos, *Air-stable all-inorganic nanocrystal solar cells processed from solution*, Science, 310, 462 (2005); https://doi.org/10.1126/science.1117908.
[19] P. Prabhakaran, W.J. Kim, , K.-S. Lee, P.N. Prasad, *Quantum dots (QDs) for photonic applications*, Opt. Mater. Express, 2, 578 (2012); https://doi.org/10.1364/Ome.2.000578
[20] S.A. McDonald et al., *Solution-processed PbS quantum dot infrared photodetectors and photovoltaics*, Nat. Mater., 4, 138 (2005); https://doi.org/10.1038/nmat1299.
[21] O.L. Lazarenkova, A.A. Balandin, *Miniband formation in a quantum dot crystal*, Journal of Applied Physics, 89(10), 5509 (2001); https://doi.org/10.1063/1.1366662].
[22] O.L. Lazarenkova, A.A. Balandin, *Electron and phonon energy spectra in a three-dimensional regimented quantum dot superlatice*, Phys. Rev. B, 66, 245319 (2002); https://doi.org/10.1103/PhysRevB.66.245319.
[23] I. Bilynskyi, R. Leshko, H. Metsan, I. Shevchuk, *Hole States in Spherical Quantum Nanoheterosystem with Intermediate Spin-Orbital Interaction*, Physics and Chemistry of Solid State, 20(3), 227 (2019); https://doi.org/10.15330/pcss.20.3.227-233.
[24] G.B. Grigoryan, E.M. Kazaryan, Al.L. Efros, T.B. Yazeva, Solid State Phys., 32(6), 1722 (1990)
[25] J.M. Luttinger and W. Kohn, *Motion of Electrons and Holes in Perturbed Periodic Fields*, Phys. Rev., 97 (4), 869 (1955).
[26] E. Menéndez-Proupin and C. Trallero-Giner, *Electric-field and exciton structure in CdSe nanocrystals*, Phys. Rev. B, 69, 125336 (2003); https://doi.org/10.1103/PhysRevB.69.125336.
[27] R.Ya. Leshko, I.V. Bilynskyi, *The hole energy spectrum of an open spherical quantum dot within the multiband model*, Physica E, l (110), 10 (2019); https://doi.org/10.1016/j.physe.2019.01.024.

І.В. Білинський, Р.Я. Лешко, Г.Я. Бандура

Електронно-дірковий спектр з урахуванням деформації та поляризації у квантовій точці гетероструктури InAs/GaAs

Дрогобицький державний педагогічний університет імені Івана Франка, м. Дрогобич, Україна,
galinka.bandura@gmail.com

У роботі досліджено сферичні квантові точки InAs в матриці GaAs. Енергії електронів і дірок в одно- і багатозонних моделях (із сильною, слабкою і проміжною спін-орбітальною взаємодією) розраховано з урахуванням як деформації матриці квантових точок, так і поляризаційних зарядів на поверхні квантових точок. . Розглянуто залежність енергетичних рівнів електронів і дірок від радіуса квантової точки. Показано, що для електрона ефекти деформації сильніші, ніж поляризація. Для дірок ці ефекти протилежні. Енергії електронів і дірок порівнювалися в усіх моделях наближення.

Ключові слова: обмінна взаємодія, деформація, 4-зонна модель або багатозонна діркова модель, 6-зонна модель, поляризаційні заряди, напружений гетеросис.