ISSN 1063-7826, Semiconductors, 2018, Vol. 52, No. 5, pp. 551–553. © Pleiades Publishing, Ltd., 2018.

XXV INTERNATIONAL SYMPOSIUM
"NANOSTRUCTURES: PHYSICS AND TECHNOLOGY",
SAINT PETERSBURG, RUSSIA, JUNE 26–30, 2017.
EXCITONS IN NANOSTRUCTURES

Calculation of Energy States of Excitons in Square Quantum Wells[1]

P. A. Belov

Department of Computational Physics, St. Petersburg State University, St. Petersburg, 198504 Russia

e-mail: pavelbelov@gmail.com

Received December 25, 2017

Abstract—The ground and excited energy states of excitons in single square GaAs-based quantum wells are found by the numerical solution of the three-dimensional Schrödinger equation. This equation is obtained within the envelope-function formalism from the exciton energy operator using the spherical approximation of the Luttinger Hamiltonian. Precise results for the exciton states are achieved by the finite-difference method. The radiative decay rates of the calculated states are also determined.

DOI: 10.1134/S1063782618050032

INTRODUCTION

Theoretical studies of the exciton states and the radiative decay rate are crucially important for interpretation of the experimental results [1]. Measurements of the radiative decay rate for high-quality quantum wells (QWs) show a variance of the results [2, 3] especially for narrow QWs. Meanwhile, the quality of heterostructures is permanently growing and new data on exciton-light coupling have become available recently [4, 5]. These recent data include the radiative decay rates for the ground and excited states of excitons in QWs.

The theoretical description of the exciton states in heterostructures is complicated by the degenerate valence band in the GaAs-based heterostructures. The impact of the QW potential additionally impedes the solution. The problem can be solved analytically only in the limiting cases of very narrow or very wide QWs ($L < 10$ nm and $L > 150$ nm for the GaAs QWs) [1]. On the other hand, recent increase of the computer performance has opened up an opportunity for numerical study of exciton states as well as of the exciton-light coupling for various widths of QWs. Nevertheless, the numerical solution by the variational method [6, 7] is mainly restricted to the exciton ground state. The excited states are difficult to be obtained by the variational method.

We have developed a method for the precise numerical solution of the Schrödinger equation for the envelope-function of an exciton in a single square QW of a finite height [8, 9]. This equation is obtained from the exciton energy operator using the spherical approximation of the Luttinger Hamiltonian [10]. Due to the reduced symmetry of the problem, one can separate only three out of the six coordinates. Then, the obtained three-dimensional equation is solved by the finite-difference method [11]. As a result, the energies of the ground and excited exciton states and corresponding wave functions depending on the remaining three coordinates have been determined. The latter allowed us to calculate the radiative decay rate, Γ_0, with a good precision for various widths of QWs. In the present report, we describe results of our calculations of $1s$-like exciton states for a heterostructure with $GaAs/Al_{0.3}Ga_{0.7}As$ QW.

THEORETICAL MODEL

The exciton states in a single square QW are defined by the three-dimensional partial differential equation derived from the Schrödinger equation for the exciton. For description of the degenerate valence band, the spherical approximation of the Luttinger Hamiltonian [10] is used, thus neglecting the corrugation of the valence band. Additionally, the light-hole-heavy-hole mixing is disregarded. This three-dimensional equation for s-wave exciton states is given as [8]

$$\left(K - \frac{e^2}{\epsilon\sqrt{\rho^2 + (z_e - z_h)^2}} + V_e(z_e) + V_h(z_h)\right) \times f(z_e, z_h, \rho) = E_X f(z_e, z_h, \rho), \quad (1)$$

where the kinetic term reads

$$K = -\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_e^2} - \frac{\hbar^2}{2m_{hz}}\frac{\partial^2}{\partial z_h^2} - \frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial \rho^2} - \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\right). \quad (2)$$

[1]The article is published in the original.

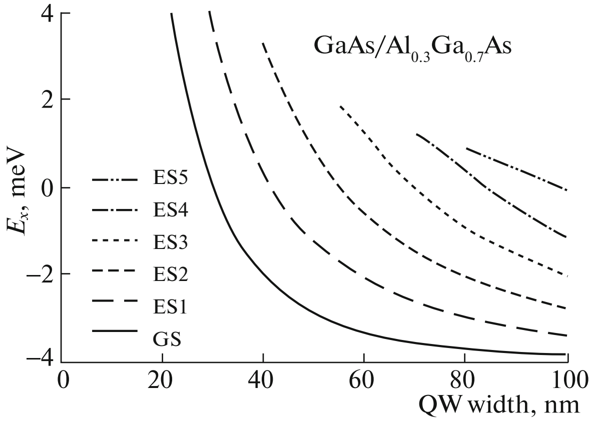

Fig. 1. The calculated energies of 1*s*-like heavy-hole states of the exciton in $GaAs/Al_{0.30}Ga_{0.70}As$ single square QW. The label "GS" denotes the ground state, whereas "ES" marks the excited states.

In the equations, indices *e* and *h* denote the electron and the hole, respectively. The unknown function f is related to the three-dimensional wave function φ as [8, 9] $\varphi(z_e, z_h, \rho) = f(z_e, z_h, \rho)/\rho$, where $\rho = \sqrt{(x_e - x_h)^2 + (y_e - y_h)^2}$. The potentials $V_{e,h}(z_{e,h})$ are the finite square confinement QW potentials. The term μ is the reduced effective mass in the *xy*-plane, m_{hz} is the hole mass in the *z*-direction. The exciton binding energy, E_b, is defined by the exciton ground state energy, E_X, with respect to the lowest quantum confinement energies of the electron, E_{e1}, and the hole, E_{h1}, in the QW: $E_b = E_{e1} + E_{h1} - E_X$. Energies E_{e1} and E_{h1} are obtained from solution of the corresponding one-dimensional Schrödinger equations for the electron and the hole in the QW.

The exciton-light coupling is usually characterized by the radiative decay rate, Γ_0, which describes the resonance response of an exciton exposed to the electromagnetic excitation. For the exciton in a QW, the radiative decay rate is given by the expression [1]:

$$\Gamma_0 = \frac{2\pi q}{\hbar\epsilon}\left(\frac{e|p_{cv}|}{m_0\omega_0}\right)^2 \left|\int_{-\infty}^{\infty}\varphi(z, z, 0)e^{iqz}dz\right|^2. \quad (3)$$

Here, $z = z_e = z_h$, $q = \omega\sqrt{\epsilon}/c$ is the light wave vector, ω_0 is the exciton frequency, $|p_{cv}|$ is the matrix element of the momentum operator between the single-electron conduction- and valence-band states.

We have numerically solved the boundary value problem for the three-dimensional partial differential equation and accurately obtained energies of the exciton states and the corresponding wave functions. The exponential decrease of the wave functions at large values of variables allowed us to impose zero boundary conditions for the function $f(z_e, z_h, \rho)$ at the boundary of some rectangular domain.

For discretization we employed the second-order finite-difference approximation [11, 12] of the partial derivatives in the three-dimensional equation on the equidistant grids over three variables. The nonzero solution of this homogeneous equation with zero boundary conditions can be found by diagonalization of the matrix constructed from this equation. A small part of the matrix spectrum was obtained by the Arnoldi algorithm [13]. As a result, we have calculated some lowest eigenvalues of the matrix and the corresponding eigenvectors. Then, the radiative decay rate was calculated using the trapezoidal rule for computing the integral for Γ_0.

The calculations were performed for heavy-hole excitons in the $GaAs/Al_{0.3}Ga_{0.7}As$ heterostructures. In particular, the difference of the gap energies of the heterostructure was modeled as $\Delta E_g = 1087x + 438x^2$ meV; a ratio of potential barriers: $V_e/V_h = 65/35$; the Luttinger parameters are taken to be $\gamma_1 = 6.85$, $\gamma_2 = 2.10$ for GaAs and $\gamma_1 = 3.76$, $\gamma_2 = 0.82$ for AlAs; the dielectric constant $\epsilon = 12.53$ for GaAs and $\epsilon = 10.06$ for AlAs [7, 14]. Masses and dielectric constants for the ternary alloys are obtained by a linear interpolation on *x*.

RESULTS

The energies of the exciton states and the radiative decay rates in energy units, $\hbar\Gamma_0$, have been calculated for QW widths $L = 20 - 100$ nm. In Fig. 1, the energies E_X (with respect to E_g) of exciton 1*s*-like states below the sum of the lowest quantum confinement energies of the electron and the hole, $E_{e1} + E_{h1}$, are shown. The number of exciton states is increased as the QW becomes wider. The ground exciton state (GS) takes place for any QW widths. The first excited state (ES1) initially appears at the minimum QW width of 25 nm with the exciton energy $E_X \approx 7$ meV (beyond the canvas of the Fig. 1). For narrow QWs, this state can be approximated by the product of three one-dimensional wave functions. They correspond to the first excited quantum-confined state of the hole, the ground quantum-confined state of the electron and the Coulomb 1s-like state. For wide QWs, the upper states for QWs of width $L > 80$ nm are difficult to be distinguished and require more precise computations.

The calculated radiative decay rates in the energy units, $\hbar\Gamma_{0n}$, for the four lowest exciton states, $n = 1 - 4$, are given in Table 1. For the upper states at the QW widths $L \geq 80$ nm, the radiative decay rates seem to be less than 1 μeV. The radiative decay rate of the first excited state ($\hbar\Gamma_{02}$) becomes noticeable only for wide QWs. As a result, in the theoretical calcula-

Table 1. The radiative decay rates of the four lowest 1*s*-like heavy-hole states of the exciton in the $GaAs/Al_{0.30}Ga_{0.70}As$ single square QW of different QW widths.

QW width (nm)	$\hbar\Gamma_{01}$ (μeV)	$\hbar\Gamma_{02}$ (μeV)	$\hbar\Gamma_{03}$ (μeV)	$\hbar\Gamma_{04}$ (μeV)
20	35	–	–	–
30	36	1	–	–
40	38	2	1	–
60	45	6	5	1
80	52	13	7	5
100	58	23	5	9

tions of Γ_{0n}, it is enough to consider only the ground exciton state, thus to neglect mixing of the states by means of the electric field of the light wave [15]. In experimental studies of the exciton-light coupling in high-quality heterostructures with GaAs/AlGaAs QWs of corresponding widths, one should observe at least the resonance response of the exciton ground state. Indeed, the numerical results are consistent with the experimental data for QW width of 20 nm presented in [8] as well as for QW width of 12 nm given in [16].

For narrow QWs ($L < 25$ nm), only the ground state takes place. According to the table, the strength of the exciton-light interaction corresponding to the ground state (and upper states) decreases as L diminishes. That means that the most long-lived exciton in the $GaAs/Al_{0.3}Ga_{0.7}As$ QW is found to be for QW widths $L \leq 30$ nm where $\hbar\Gamma_0$ is smaller. The accurate modeling of exciton states for such QW widths, however, should take into account the discontinuities of the material parameters at the interfaces.

CONCLUSION

In summary, we calculated the ground and excited energy states of the heavy-hole exciton in a single square $GaAs/Al_{0.3}Ga_{0.7}As$ QWs of various QW widths. The numerical solution was performed using the finite-difference approximation of the three-dimensional Schrödinger equation and exact diagonalization of the obtained matrix equation. The radiative decay rates of the calculated 1*s*-like states were determined. It is shown that the ground state has the largest radiative decay rate. The numerical results are consistent with the experimental data for QW width of 20 nm presented in [8] as well as for QW width of 12 nm given in [16].

ACKNOWLEDGMENTS

The work is supported by SPbU (grants nos. 11.38.213.2014, 11.38.241.2015), RFBR (grants nos. 16-02-00245, 16-32-00047) and DFG in the frame of Project ICRC TRR 160. The calculations were carried out using the facilities of the SPbU Resource Center "Computational Center of SPbU".

REFERENCES

1. E. L. Ivchenko, *Optical Spectroscopy of Semiconductor Nanostructures* (Alpha Science, Harrow, 2005).
2. S. V. Poltavtsev and B. V. Stroganov, Phys. Solid State **52**, 1899 (2010).
3. S. V. Poltavtsev, Yu. P. Efimov, Yu. K. Dolgikh, et al., Solid State Commun. **199**, 47 (2014).
4. D. K. Loginov, A. V. Trifonov, and I. V. Ignatiev, Phys. Rev. B **90**, 075306 (2014).
5. A. V. Trifonov, S. N. Korotan, A. S. Kurdyubov, et al., Phys. Rev. B **91**, 115307 (2015).
6. D. B. T. Thoai, R. Zimmermann, M. Grundmann, and D. Bimberg, Phys. Rev. B **42**, 5609(R) (1990).
7. B. Gerlach, J. Wüsthoff, M. O. Dzero, and M. A. Smondyrev, Phys. Rev. B **58**, 10568 (1998).
8. E. S. Khramtsov, P. A. Belov, P. S. Grigoryev, et al., J. Appl. Phys. **119**, 184301 (2016).
9. P. A. Belov and E. S. Khramtsov, J. Phys.: Conf. Ser. **816**, 012018 (2017).
10. J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).
11. A. A. Samarskii, *The Theory of Difference Schemes* (Nauka, Moscow, 1989) [in Russian].
12. S. Glutsch, *Excitons in Low-Dimensional Semiconductors* (Berlin, Springer, 2004).
13. R. B. Lehoucq, D. C. Sorensen, and C. Yang, *ARPACK Users' Guide: Solution of Large-Scale Eigenvalue Problems with Implicitly Restarted Arnoldi Methods* (SIAM, Philadelphia, 1997).
14. I. Vurgaftman, J. R. Meyer and L. R. Ram-Mohan, J. Appl. Phys. **89**, 5815 (2001).
15. M. M. Voronov, E. L. Ivchenko, V. A. Kosobukin and A. N. Poddubny, Phys. Solid State **49**, 1792 (2007).
16. Y. Chen, N. Maharjan, Z. Liu, et al., J. Appl. Phys. **121**, 103101 (2017).