EAST EUROPEAN JOURNAL OF PHYSICS. 4. 307-310 (2023)
DOI:10.26565/2312-4334-2023-4-40 ISSN 2312-4334

TO THE THEORY OF DIMENSIONAL QUANTIZATION IN NARROW-GAP CRYSTALS

Sharifa B. Utamuradova[a], Rustam Y. Rasulov[b], Voxob R. Rasulov[b], Kamolakhon K. Urinova[b], Kakhramon M. Fayzullaev[a]*

[a] *Institute of Semiconductor Physics and Microelectronics at the National University of Uzbekistan, Tashkent, Uzbekistan*
[b] *Fergana State University, Fergana, Uzbekistan*
**Corresponding Author e-mail: qahramonfayzullaev8@gmail.com*
Received October 7, 2023; revised November 13, 2023; accepted November 15, 2023

This article discusses studies of size quantization phenomena in zero-, one-, and two-dimensional semiconductor structures. The main attention is paid to the mechanisms of photon-kinetic effects in these structures. Despite many studies of the physical properties of low-dimensional systems of current carriers, the size quantization of energy spectra in narrow-gap semiconductors and the associated photonic-kinetic effects are still insufficiently studied. Therefore, this study focuses on the quantum mechanical study of size quantization in certain cases using Kane's multiband model. The insolvability of the 8×8 matrix Schrödinger equation in the Kane model for a potential well of arbitrary shape is analyzed. The dependence of the energy spectrum on the two-dimensional wave vector is studied for various cases. In particular, the energy spectra for InSb and GaAs semiconductors are considered, depending on the band parameters and the size of the potential well. Conclusions are presented on the analysis of various cases of size quantization in narrow-gap crystals with cubic or tetrahedral symmetry in the three-band approximation. It is shown that the energy spectrum corresponds to a set of size-quantized levels that depend on the Rabi parameter, band gap, and well size. The size-quantized energy spectra of electrons and holes in InSb and GaAs semiconductors are analyzed in a multiband model.
Keywords: *Dimensional Quantization; Narrow-Gap; Crystal; Kane model; Schrödinger equation; Electron; Subband; Nanoelectronics; Heterostructure; Energy spectrum*
PACS: 71.20. – b, 71.28. + d

INTRODUCTION

Modern achievements in the field of nanoelectronics and nanotechnology have made it possible to observe and study new unique phenomena occurring in zero-, one-, and two-dimensional semiconductor structures [1-5]. The creation of such structures contributes to the study of the mechanisms of photon-kinetic effects occurring in them [6-9].

Although many works [10-14] are devoted to the study of physical properties of low-dimensional systems of current carriers, but dimensional quantization of energy spectra in narrow-gap semiconductors and related photon-kinetic effects are rather poorly investigated. Therefore, this paper quantum-mechanically investigates dimensional quantization in specific cases. The calculations are carried out in the multizone Kane model [3, 15, 16].

THE SCHRÖDINGER EQUATION AND ANALYSIS OF ITS SOLUTIONS FOR VARIOUS CASES

In the first part of this paper, it is shown that in the approximation of the multizone Kane model the matrix Schrödinger equation is analytically unsolvable for a potential well of arbitrary shape. Therefore, it investigates the dependence of the energy spectrum of the two-dimensional wave vector perpendicular to the direction of dimensional quantization (on the *Oz* axis) for various cases differing in the region of current carrier energy values. As in the first part, for simplification of calculations we will restrict ourselves to linear in terms of the summands in the Kane Hamiltonian, $\vec{k}$ – the wave vector of current carriers. Then the Schrödinger equation in the Kane model can be represented as:

$$\frac{\partial^2 \varphi_{1,2}}{\partial z^2} - \kappa_1^2 \varphi_{1,2} = 0, \tag{1}$$

whose solution is found in the form

$$\varphi_{1,2}(z) = c_1 e^{i\kappa_1 z} + c_2 e^{-i\kappa_1 z} \text{ or } \varphi_{1,2}(z) = d_1 \cos(\kappa_1 z) + d_2 \sin(\kappa_1 z), \tag{2}$$

where c_1, c_2- integration constants

$$\kappa_1^2 = -\frac{\Lambda_0}{\Lambda_2} = \frac{\frac{3}{P^2}\Xi_V \Xi_{gv}^2 + \left(2\Xi_{gV} + \frac{\Xi_{gV}^2}{\Xi_{g\Delta V}}\right)\cdot k_1^2}{\left(2\Xi_{gV} + \frac{\Xi_{gV}^2}{\Xi_{g\Delta V}}\right) + \left(2 + \frac{\Xi_{gV}^2}{\Xi_{g\Delta V}^2}\right)V_0} \tag{3}$$

and at $U_0 = 0$

Cite as: Sh.B. Utamuradova, R.Y. Rasulov, V.R. Rasulov, K.K. Urinova, K.M. Fayzullaev, East Eur. J. Phys. 4, 307 (2023), https://doi.org/10.26565/2312-4334-2023-4-40

$$\kappa_1^2 = \frac{3}{P^2}\frac{E(E+E_g)^2}{\left(2(E+E_g)+\frac{(E+E_g)^2}{E+E_g+\Delta}\right)} - k_\perp^2. \quad (4)$$

If in expression (2) we take into account the condition of continuity of wave functions at the interface of the heterostructure: $\varphi_{1,2}(z=0) = \varphi_{1,2}(z=a) = 0$, then the size quantization of the energy spectrum of current carriers can be analyzed for the following cases:

1-case. When a particle moves in the field of a potential well ($U_0 = 0$), then the dependence of the energy spectrum on the two-dimensional wave vector is determined by the relation:

$$k_{\perp,n_1}^2(E) = \frac{3}{P^2}\frac{E(E+E_g)^2}{\left(2(E+E_g)+\frac{(E+E_g)^2}{E+E_g+\Delta}\right)} - \left(\frac{\pi n_1}{a}\right)^2, \quad (5)$$

Figures 1 and 2 show the energy spectra for *InSb* and *GaAs*, calculated according to (5) for three size-quantized subbands. In the calculations, the following values were chosen: for the InSb crystal $m_{el} = 0.0143m_0$ - effective mass of electrons, $a = 50 \cdot 10^{-10}m$ (Fig. 1 a), $a = 75 \cdot 10^{-10}m$ (Fig. 1 b) - potential well width, $E_g = 0{,}18eV$ - band gap, $\Delta = 0.803\ eV$ - spin-orbit splitting energy, and for GaAs: $m_{el} = 0.063m_0$ - effective electron mass, $a = 50 \cdot 10^{-10}m$ (Fig. 2 a), $a = 75 \cdot 10^{-10}m$ (Fig. 2 b), $E_g = 1.52eV$, $\Delta = 0{,}341\ eV$, $P = \frac{\hbar}{2}\sqrt{\frac{3E_g}{m_{el}}}$ - Kane parameter.

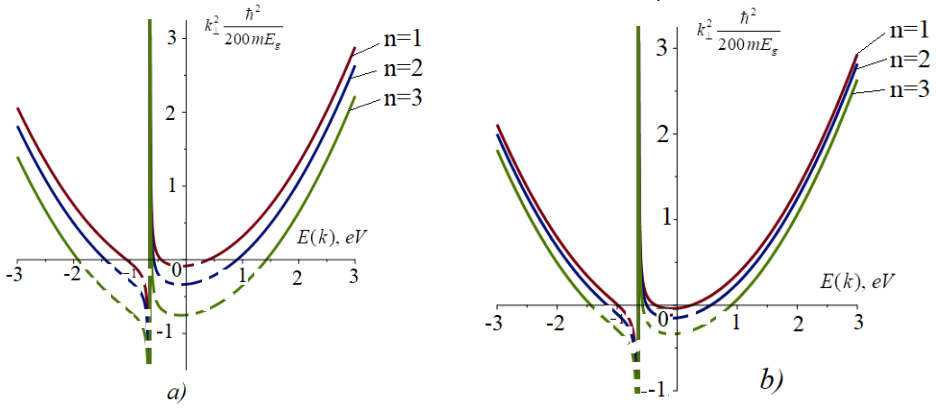

Figure 1. Size-quantized energy spectrum of electrons in InSb

In these figures, the region of negative values of the squared wave vector corresponds to the region of forbidden energies, represented by dashed lines, which represent the bandgap width and the spin-orbit splitting zone. From Fig. 1 and 2 it is clear that with increasing width of the potential well, the width of the band gap decreases (due to a shift in the energy spectrum due to size quantization) and the energy distance between close states of size quantization levels (since the energy spectrum of size quantization is inversely proportional to the width of the well).

Therefore, the energy states of electrons in the conduction band (solid line in the region of positive energy values (see Fig. 2)) and the subband of light holes in the valence band (solid line in the region of negative energy values in Fig. 2) are quantized depending on the size of the potential well, and the heavy hole subband of the valence band corresponds to a vertical line, since in Kane's approximation it does not depend on the hole wave vector. In the calculations, the minimum value of the conduction band was chosen as the energy reference point, so the electron energy is positive and the hole energy is negative.

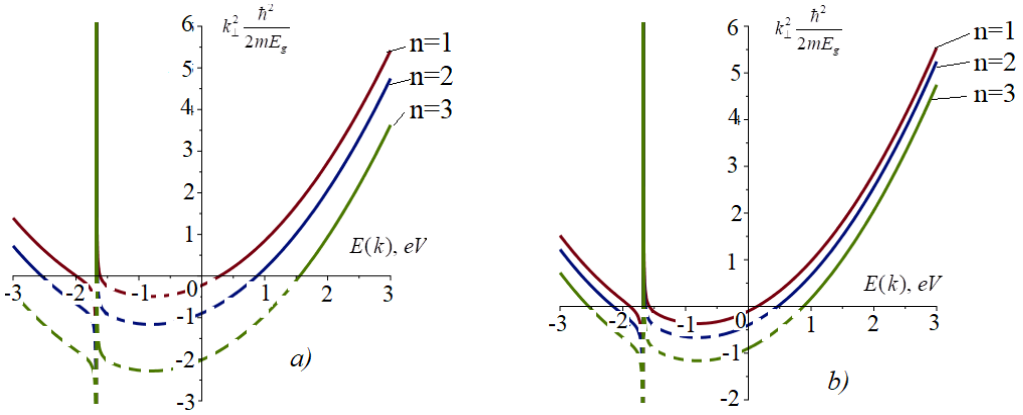

Figure 2. Size-quantized energy spectrum of electrons in GaAs

2-case. When the particle moves along the direction of dimensional quantization (in this case $k_x = 0, k_y = 0$), then the energy spectrum corresponds to a set of dimensionally quantized levels, depending on the zone parameters and the size of the hole and is described by the expression

$$\frac{\frac{3}{P^2}(E-U_0)\left(E+E_g-U_0\right)^2}{\left(2\left(E+E_g-U_0\right)+\frac{\left(E+E_g-U_0\right)^2}{E+E_g+\Delta-U_0}\right)+\left(2+\left(\frac{E+E_g-U_0}{E+E_g+\Delta-U_0}\right)^2\right)U_0}=\left(\frac{\pi n_1}{a}\right)^2, \tag{6}$$

In both - above-mentioned cases the expressions of dimensional quantization can be simplified in the following way:

(a) The energy region of current carriers satisfying the condition $E + E_g << \Delta$ is defined as

$$k^2_{\perp,n_1}(E)=\frac{3}{P^2}E\left(E+E_g\right)-\left(\frac{\pi n_1}{a}\right)^2, \tag{7}$$

from which we have an expression for the energy spectrum having two branches dimensionally quantized, which correspond to the dimensional quantization of subzones of electrons in the conduction zone (sign "+") and light holes (sign "-")

$$E_{\pm}(k_{\perp})=\frac{E_g}{2}\left\{-1\pm\sqrt{1+\frac{4P^2}{3E_g^2}\left[\left(\frac{\pi n_1}{a}\right)^2+k^2_{\perp}\right]}\right\}. \tag{8}$$

Here and below $n_1 = 1,2,\ldots$;

(b) at $E + E_g - U_0 << \Delta$ the dimensionally quantized levels are defined by the relation

$$\left(\frac{\pi n_1}{a}\right)^2=\frac{1}{P^2}\frac{(E-U_0)\left(E+E_g-U_0\right)^2}{(E+E_g)}; \tag{9}$$

(c) Under the condition $E + E_{g_0} >> \Delta$ the dependence of the current carrier energy on the two-dimensional wave vector is defined as

$$k^2_{\perp,n_1}(E)=\frac{1}{P^2}E\left(E+E_g\right)-\left(\frac{\pi n_1}{a}\right)^2, \tag{10}$$

from which we obtain the expression for the size-quantized energy spectrum of electrons (sign "+") and light holes (sign "-")

$$E_{\pm}(k_{\perp})=\frac{E_g}{2}\left\{-1\pm\sqrt{1+\frac{4P^2}{E_g^2}\left[\left(\frac{\pi n_1}{a}\right)^2+k^2_{\perp}\right]}\right\} \tag{11}$$

The energy spectrum of electron size quantization calculated for InSb by expression (11) is shown in Fig. 3, where a) for the two-dimensional case; b) for the three-dimensional case. The above values of physical quantities are chosen in the calculations;

(d) under the condition $E + E_g - U_0 << \Delta$ there appear the dimensionally quantized levels defined by the relation

$$\left(\frac{\pi n_1}{a}\right)^2=\frac{3}{2P^2}\frac{(E-U_0)\left(E+E_g-U_0\right)^2}{E+E_g}, \tag{12}$$

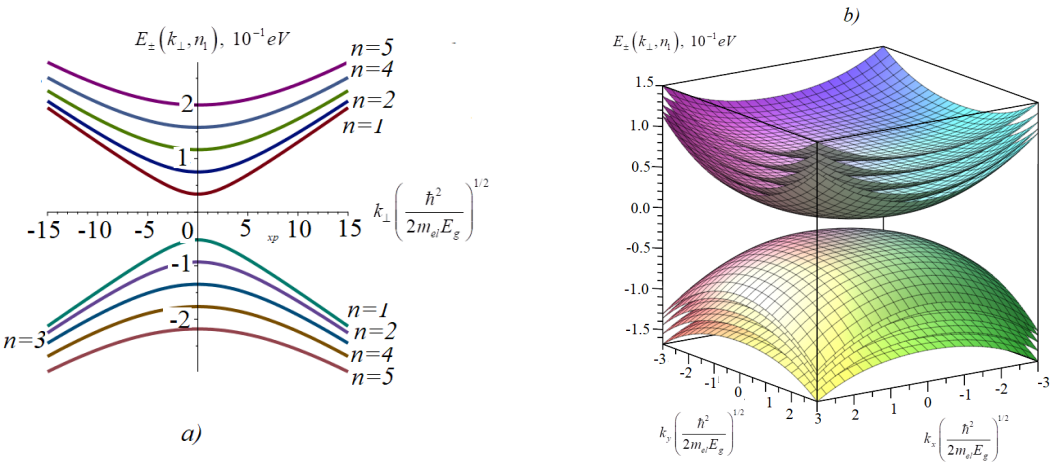

Figure 3. Size-quantized energy spectrum of electrons in InSb: a) two-dimensional; b) three-dimensional case

CONCLUSIONS

Thus, various cases of dimensional quantization in narrow-gap crystals of cubic or tetrahedral symmetry in the three-gap Kane approximation have been analyzed.

Expressions are obtained for the energy spectrum depending on the two-dimensional wave vector when electrons move both in the field of a potential well, directed along the interface of the heterostructure, and in the direction of size quantization. It is shown that in this case the energy spectrum corresponds to a set of dimensionally quantized levels, depending on the Rabi parameter, the band gap and the size of the well.

The size-quantized energy spectrum of electrons in the conduction band and holes in the subband of light holes in InSb and GaAs semiconductors was analyzed in the three-band Kane model, where the mass of heavy holes is considered infinite [15].

ORCID

Sharifa B. Utamuradova, https://orcid.org/0000-0002-1718-1122; **Rustam Y. Rasulov,** https://orcid.org/0000-0002-5512-0654
Voxob R. Rasulov, https://orcid.org/0000-0001-5255-5612; **Kakhramon M. Fayzullaev,** https://orcid.org/0000-0001-7362-1439

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ДО ТЕОРІЇ РОЗМІРНОГО КВАНТУВАННЯ У ВУЗЬКОЩІЛИННИХ КРИСТАЛАХ

Шаріфа Б. Утамурадова[a], Рустам Ю. Расулов[b], Воксоб Р. Расулов[b], Камолахон К. Урінова[b], Кахрамон М. Файзуллаєв[a]
[a]Інститут фізики напівпровідників і мікроелектроніки Національного університету Узбекистану, Ташкент, Узбекистан
[b]Ферганський державний університет, Фергана, Узбекистан

У цій статті розглядаються дослідження явищ розмірного квантування в нуль-, одно- та двовимірних напівпровідникових структурах. Основну увагу приділено механізмам фотонно-кінетичних ефектів у цих структурах. Незважаючи на численні дослідження фізичних властивостей низькорозмірних систем носіїв струму, розмірне квантування енергетичних спектрів у вузькозонних напівпровідниках і пов'язані з ним фотоніко-кінетичні ефекти ще недостатньо вивчені. Таким чином, це дослідження зосереджено на квантово-механічному дослідженні розмірного квантування в певних випадках з використанням багатозонної моделі Кейна. Проаналізовано нерозв'язність матричного рівняння Шредінгера 8x8 у моделі Кейна для потенційної ями довільної форми. Досліджено залежність енергетичного спектра від двовимірного хвильового вектора для різних випадків. Зокрема, розглянуто енергетичні спектри напівпровідників InSb та GaAs залежно від параметрів зони та розміру потенційної ями. Подано висновки щодо аналізу різних випадків розмірного квантування у вузькозонних кристалах з кубічною або тетраедричною симетрією в тризонному наближенні. Показано, що енергетичний спектр відповідає набору розмірно-квантованих рівнів, які залежать від параметра Рабі, забороненої зони та розміру ями. Розмірно квантовані енергетичні спектри електронів і дірок у напівпровідниках InSb і GaAs проаналізовано в багатозонній моделі.

Ключові слова: *вимірне квантування; вузька щілина; кристал; модель Кейна; рівняння Шредінгера; електрон; підзона; наноелектроніка; гетероструктура; енергетичний спектр*