3D self-consistent solution of Poisson and Schrödinger equations for electrostatically formed quantum dot

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Abstract. In this work we discuss 3D selfconsistent solution of Poisson and Schrödinger equations for electrostatically formed quantum dot. 3D simulations give detailed insight into the energy spectrum of the device and allow us to find values of respective voltages ensuring given number of electrons in the dot. We performed calculations for fully 3D potential and apart from that calculations for the same potential separated into two independent parts, i.e. regarding to the plane of 2DEG and to the direction perpendicular to the meant plane. We found that calculations done for the two independent parts of the potential give good information about quantum dot properties and they are much faster compared to fully 3D simulations.

Key words: quantum dot, Poisson equation, Schrödinger equation, Hartree approximation, electron-electron interaction, zero-dimensional electron gas, inverted heterostructure, ISIS.

1. Introduction

Quantum dots are nanoscale devices which may be used in many nanoelectronic applications. For example they may be treated as the memory cells which can be arranged into matrixes and form whole memory circuits. Numerical simulations performed even for a single quantum dot appear very complicated. The reason is that Poisson and Schrödinger equations must be solved to describe electronic states in such a system [1]. Both the equations must be solved numerically and must regard to the special design of the given device.

In the work we present results of simulations which were done for quantum dot formed electrostatically in an inverted heterostructure (Fig. 1) [2–4].

The structure is driven by voltages U_{GS} and U_{ES} polarizing respective electrodes. Suitable value of U_{GS} allows to create two-dimensional electron gas (2DEG) in GaAs region very close to GaAs/AlGaAs heterojunction. The voltage U_{ES} eliminates created 2DEG in the region under the splitted, upper electrode E. This way, in the central part of the structure, a quantum dot is formed. In order to describe the potential distribution over the structure we performed the numerical solution of Poisson equation in 3D space.

Looking for electron states in the device relies on finding of Schrödinger equation solutions. We did it for fully three-dimensional potential distribution. 3D Poisson and Schrödinger equations were solved self-consistently.

Three-dimensional model of the structure is quite demanding because of computational complexity and request for large computer memory. Our aim was to check up if the approach in which electron gas is treated sep-

arately in a plane of 2DEG (x-y plane) and separately in z direction (perpendicular to a heterojunction), can provide acceptable results. To reach the aim we had to perform simulations in the other way – treating electron gas in a mentioned above simplified manner. We solved one-dimensional Schrödinger equation for the part of potential distribution corresponding to z direction. As a result we obtained the ground state of 2DEG together with the electron gas density distribution. We verified how far from a heterojunction there was the maximum of the calculated electron gas density. In the stated xy plane we performed self-consistent solution of 2D Poisson and Schrödinger equations. Superposition of the results obtained for 1D and 2D problems gave final information which could be compared with the results obtained in fully three-dimensional simulations.
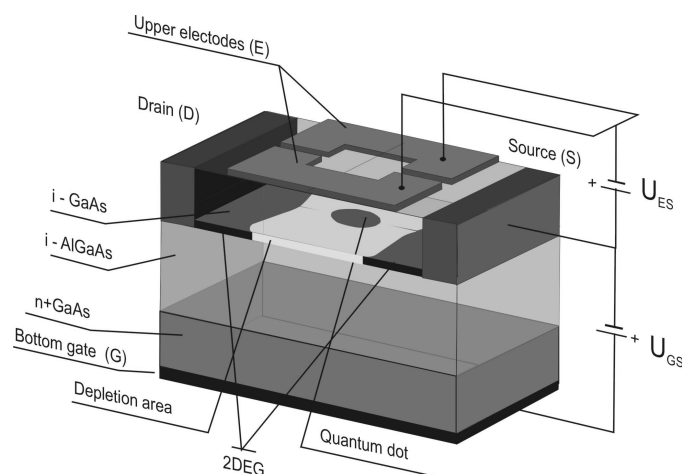

Fig. 1. The model of analyzed device

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2. Numerical model and the simulation method

Numerical analysis of the problem requires solving of Poisson equation for the device:

$$\Delta V\left(\mathbf{r}\right) = -\frac{\rho\left(\mathbf{r}\right)}{\varepsilon}, \qquad \mathbf{r} = (x, y, z) \qquad (1)$$

where ρ denotes electrical charge density in the region of 2DEG, describing electron gas outside the quantum dot (i.e. in two regions neighbouring with source and drain – Fig. 1). During the analysis, we specified the values of the potential in the five conductive regions. These regions are metallic electrodes: G, D, S and the splitted electrode E. Two undoped semiconductor layers (i.e., AlGaAs and GaAs) are treated as dielectrics with different permitivities – ε_1 and ε_2, respectively. We solved Eq. (1) assuming boundary conditions concerning constant potential over the surfaces of five mentioned electrodes and in the region of 2DEG. At the interface of non-doped AlGaAs and GaAs layers we have also assumed the continuity of the potential and of the normal component of electrical induction. Because charge density ρ is not known function, numerical solution of the Eq. (1) had to be performed in a self-consistent manner.

The function $V\left(\mathbf{r}\right)$ was searched for in the form of single layer potentials:

$$V_i(p_i) = \frac{1}{4\pi\varepsilon_i} \int\limits_{S_i} \frac{\sigma_{S_i}}{|\mathbf{r}|} ds_i, \qquad (2)$$

$$\text{where: } i = \begin{cases} 1 - \text{ for AlGaAs region} \\ 2 - \text{ for GaAs region} \end{cases}$$

In the Eq. (2) σ_{S_i} describe charge densities corresponding to single layer potentials at the surfaces S_i, which define the boundaries of i-th region. In the same equation $\mathbf{r} \equiv (x, y, z)$ is the distance between any point p_i of i-th region and any point laying on the boundary surfaces of the region. To solve the Eqs. (1) and (2) we used boundary element method and Gauss method dedicated for sets of linear equations [4]. As a result we have obtained three-dimensional potential distribution over the investigated structure.

Suitable potential formation in the plane of electron gas gives the possibility to create a quantum dot in a central part of the structure. We looked for charge density in the dot applying quantum mechanical formalism. Energy levels E and wave functions $\Psi\left(\mathbf{r}\right)$ describing electrons in a dot, fulfill Schrödinger Eq. [5]:

$$-\frac{\hbar^2}{2m_{GaAs}^{*\Gamma}}\Delta\Psi\left(\mathbf{r}\right) + e\left[V\left(\mathbf{r}\right) + V_H\left(\mathbf{r}\right)\right]\Psi\left(\mathbf{r}\right) = E\Psi\left(\mathbf{r}\right) \quad (3)$$

Potential $V\left(\mathbf{r}\right)$ has the origin from voltages biasing the device. Electron's effective mass $m_{GaAs}^{*\Gamma}$ corresponds to the minimum Γ in GaAs layer. Interactions among N electrons in the quantum dot were described by Hartree potential $V_H\left(\mathbf{r}\right)$:

$$V_H(\mathbf{r}) = \sum_{j}^{1,N} \int\limits_{\Omega} \frac{e \, |\Psi_j(\mathbf{r}_j)|^2}{4\pi\varepsilon \, |\mathbf{r} - \mathbf{r}_j|} \, d\Omega. \qquad (4)$$

In the case of true three-dimensional analysis $\mathbf{r} = (x, y, z)$. Wave function $\Psi_j\left(\mathbf{r}_j\right)$ describes the j-th electron in the well ($j = 1, \ldots, N$) and corresponds to the appropriate energy level of the whole spectrum E.

The charge accumulated in the dot (expressed as $\sum_{j}^{1,N} |\Psi_j(\mathbf{r}_j)|^2$) influences potential distribution over the structure. Because of that Eqs. (3) and (1) must be solved iteratively until charge and potential distributions don't change in succesive iterations.

In this work we report simulations performed with fully three-dimensional model of the device. We present obtained energy spectrum $E \equiv E_{x,y,z}$ and charge density in the dot determined with the help of calculated wavefunctions $\Psi\left(x, y, z\right)$.

In the paper we also discuss three-dimensional results obtained in the other and much faster way. To obtain them we have solved one-dimensional Schrödinger equation in the form:

$$-\frac{\hbar^2}{2m_{GaAs}^{*\Gamma}}\Delta\Psi\left(z\right) + eV\left(z\right)\Psi\left(z\right) = E_z\Psi\left(z\right). \qquad (5)$$

It allowed us to find energy levels E_z appearing due to confining of electron's motion in z direction. Localization of the lowest energy level E_{z1} (related to the potential of source $V_S = 0$) indicates whether the value of U_{GS} is sufficient to form electron gas in the dot. Energy E_{z1} fulfills Eq. (5) together with wave function $\Psi_1\left(z\right)$. We have found the maximum of $\Psi_1\left(z\right)$ and indicated how far from a heterojunction the electron gas should be analyzed if it is treated as two-dimensional. Over the discovered x-y plane we determined the potential distribution $V\left(x, y, z = const.\right)$ and we solved Eq. (3) in 2D space [6]. This way we obtained supplemental information about electron states in the dot, i.e. energy spectrum $E \equiv E_{x,y}$ and wave functions $\Psi\left(x, y\right)$. In order to state occupied energy levels in the dot energies $E_{x,y}$ were shifted by the value of E_{z1}. In the case of wavefunctions we formed products of ground state wavefunction $\Psi\left(z\right)$ with $\Psi\left(x, y\right)$ wavefunctions refering to subsequent $E_{x,y}$ levels.

In the work we compare results of 3D simulations obtained with the help of both described methods. This was the primary aim of our work. However, particular simulations gave us also the opportunity to conclude about arising of zero-dimensional electron gas in different biasing conditions.

3. Results

We performed simulations for the structure with characteristic dimensions as illustrated in Fig. 2.

Calculations were done for biasing voltages: $U_{GS} = 557$ mV, $U_{ES} = -220$ V and $U_{DS} = 0$ V. There were considered different permitivities of GaAs and AlGaAs layers (13,2 and 12,8 respectively). We solved Eq. (2) in three dimensions. As a result we found potential distribution $V\left(x, y, z\right)$ over the structure. In order to find charge den-

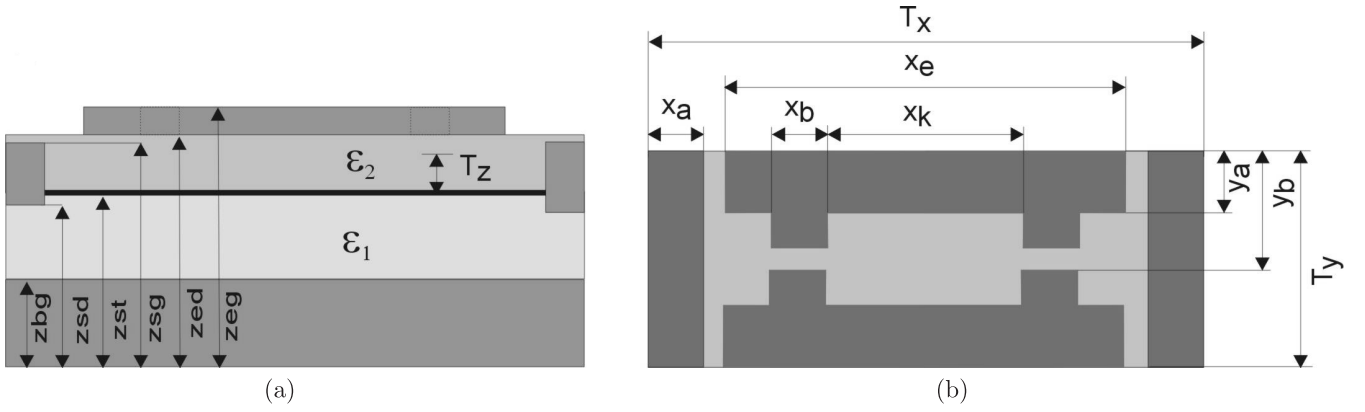(a)   (b)

Fig. 2. (a) Side view and b) top view of the device. In both figures there are marked sizes of the structure. In calculations there were taken the following values of respective dimensions (expressed in nm): zeg = 700, zed = 670, zsg = 620, zst = 600, zsd = 580, zbg = 300, $T_x = 800$, $T_y = 400$, $x_a = 50$, $x_b = 150$, $x_k = 400$, $x_e = 600$, $y_a = 50$, $y_b = 200$

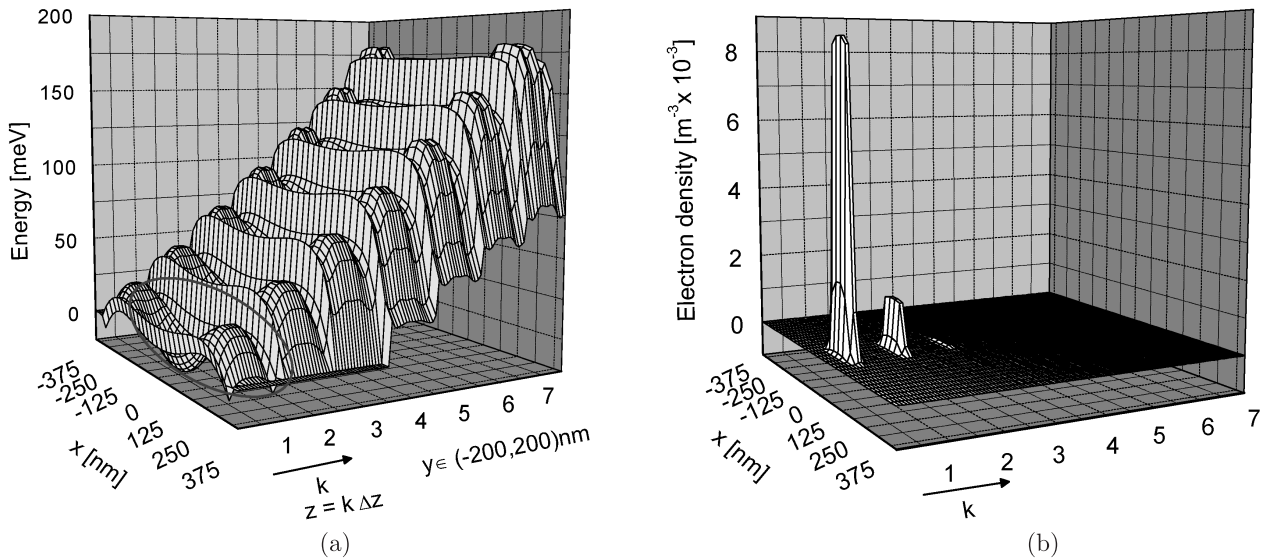(a)   (b)

Fig. 3. (a) Potential energy in 3D space, obtained from Eq. (2) and taken into account in Eq. (3). There are shown 7 dependencies $eV(x, y, z = const.)$ for 7 values $z = k\Delta z$ where $\Delta z = 10$ nm. In every illustrated dependence $eV(x, y, z = const.)$ coordinate y changes in the interval of $-200 \div 200$ nm. Quantum well referring to $k = 1$ (marked with the circle) corresponds to maximum of electron density in the dot and it is considered in Eq. (3) in 2D space. b) Charge density distribution for four electrons in the dot, corresponding to three-dimensional potential energy in Fig. (a)

sity in the dot we analyzed the region of dimensions: $T_x = 800$ nm, $T_y = 400$ nm and $T_z = 70$ nm (Fig. 2b, 2a). In true 3D simulations we found that the maximum of charge density occurs at the distance of 10 nm from GaAs/AlGaAs contact (Fig. 3b). Calculations were performed with the discretization mesh $32 \times 16 \times 7$. For such case the matrix of Hamiltonian required almost 100 MB of the computer operating memory. The whole selfconsistent analysis lasted 103 hours.

Further simulations for the device we did in a simplified manner. We solved Eq. (5) with the potential $V(z) \equiv V(0, 0, z)$. Calculated energy levels E_{z1}, E_{z2} and wave function $\Psi_1(z)$ for the lowest energy level are shown in Fig. 4b. We stated that only the base level E_{z1} is lying below reference energy which is equal to 0. More-

over, in Fig. 4b we can see that the maximum of charge density distribution appears at the same distance from heterojunction as we have stated earlier in fully three-dimensional simulations (i.e. 10 nm from GaAs/AlGaAs contact). Localization of the base energy level, below reference energy, denotes that there is fulfilled fundamental condition for the existence of electron gas in the dot.

In the next step of simulations we calculated energy levels $E_{x,y}$ and wave functions $\Psi(x, y)$ for the potential $V(x, y) = V(x, y, z = 10nm)$. Obtained energies $E_{x,y}$ were added to the value of E_{z1} and this way we got the spectrum which could be compared to energies $E_{x,y,z}$ calculated from Eq. (3) in truly 3D space.

In Fig. 4a there are shown energy levels $E_{x,y,z}$ and $E_{x,y} + E_{z1}$ obtained by the solution of Schrödinger equa-

tion including coulomb interaction among 4 electrons in the dot. In the figure there are also shown differences $E_{x,y,z} - (E_{x,y} + E_{z1})$ for particular level numbers. The differences are nearly the same as ΔE_{z1}, which expresses the change of E_{z1} caused by interaction among electrons in the dot.

Figure 4b presents quantum well in z direction together with energy levels $E_{z1} = -8.12$ meV and $E_{z2} = 5.90$ meV. Both mentioned energies and presented in the same figure charge density distribution $\rho(z)$ were obtained by solving of Eq. (5).

In the simplified analysis the 1D problem (in z direction) was described by the use of the discretization mesh with the same number of nodes as for fully 3D calculations. Hamiltonian was represented by a matrix of only 49 elements and therefore energies E_z and wavefunctions $\Psi(z)$ were found just immediately. Additionally it was tested that the same calculations performed with the mesh containing 70 nodes ($\Delta z = 1$ nm) took only 2 seconds.

The results of 2D analysis were obtained with the discretization mesh which contained 32×16 nodes. In this case the matrix of Hamiltonian was stored in only 2MB of the computer memory. Furthermore, these calculations were done within only 12 minutes.

Validity of the '2D+1D' analysis can be confirmed by the results of measurements. Experimental spectra obtained for the arrays of quantum dots were presented in the works [7,8]. The dots formed in squares of 500×500 nm² and smaller ones were measured with the help of far-infrared (FIR) spectroscopy. It was found that the spacing between successive energy levels in these dots took the values of only a few meV. On the other hand, the separation between the quantized energy levels E_z being the consequence of the conduction band non-continuity, is much greater. In the devices which take the advantage of the hetero-interface (including quantum dots) only the lowest level E_{z1} is occupied. The next level E_{z2} lies a dozen of meV above E_{z1} [9].

The above discussion shows that the constriction of electron's motion in z direction is much stronger than in x-y plane. This is the reason for which the system may be analyzed separately in the plane of 2DEG and in the direction perpendicular to the heterointerface.

4. Summary and conclusion

The results presented in this work are partial results of the project, the aim of which is to create the simulator for single electron transistor formed in ISIS structure. Numerical complexity of calculations and necessity to process big matrices, which describe three-dimensional model of the device motivated efforts for searching more optimal solutions with respect to computational time as well as precision of calculations.
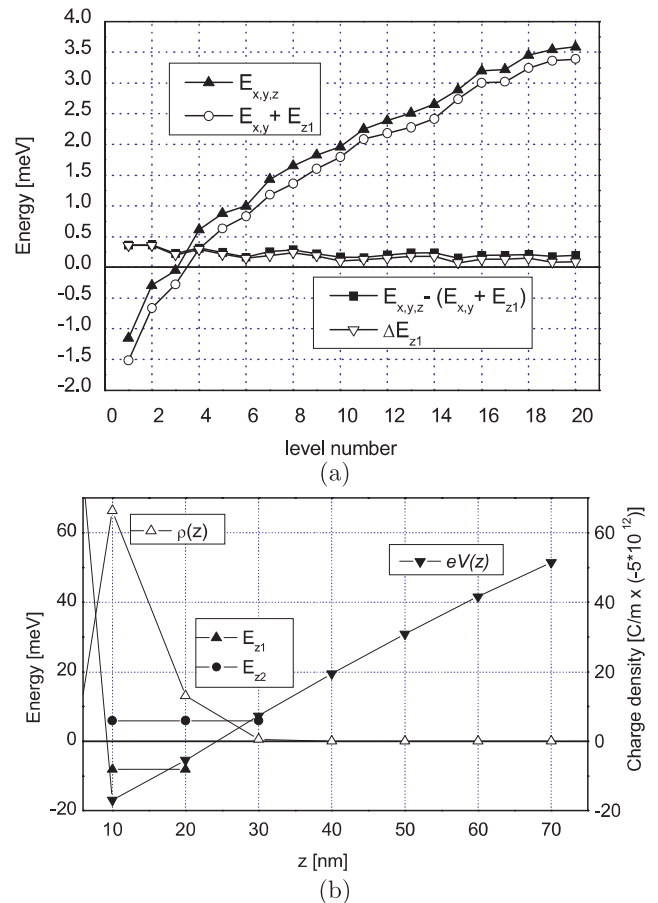

(a)

(b)

Fig. 4. (a) Energy levels $E_{x,y,z}$ calculated in fully 3D simulations are compared to energies obtained as a sum of values $E_{x,y}$ and E_{z1} gained in 2D and 1D simulations, respectively. During simulations coulomb interaction among 4 electrons in the well was taken into account. In the figure there are also shown differences $E_{x,y,z} - (E_{x,y} + E_{z1})$ for particular level numbers. The differences are nearly the same as ΔE_{z1}, which expresses the change of E_{z1} caused by interaction among electrons in the dot. (b) There is shown the quantum well in z direction, described as $eV(z)$. Energy levels $E_{z1} = -8.12$ meV and $E_{z2} = 5.90$ meV are marked in the well. In the figure there is also presented charge density distribution $\rho(z)$ obtained by solving of Eq. (5)

Calculated potential distribution in 3D space (Fig. 3a) proves that Schrödinger equation may be considered separately in the direction perpendicular to heterojunction and in the plane of 2DEG. Such treatment of self-consistent solution of Poisson and Schrödinger equation allows for substantial accelerating simulations comparing to the analysis in 3D space. However, the results of '2D+1D' calculations have to be analyzed with great care, in particular with regard to positions of energy levels, which determine the number of electrons in quantum dot for a given electrode potentials. The agreement between two methods has been demonstrated, providing that the identical discretization schemes have been used.

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