

MODELING OF ELECTRONIC STATES OF A SINGLE DONOR IN MIS-STRUCTURE USING THE FINITE DIFFERENCE METHOD

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Abstract: Numerical modeling of electronic state evolution due to external electric field in the structure metal-insulator-semiconductor with solitary donor center is carried out. Considering a nanometer disc-shaped gate as a source of the electric field, the problem for the Laplace equation in infinite multilayered medium is solved to determine the gate potential. The energy spectrum of a bound electron is calculated from the problem for the stationary Schrödinger equation. Finite difference schemes are constructed to solve both the problems. Difference scheme for the Schrödinger equation takes into account cusp condition for the wave function at the donor location. To solve the problem for the Laplace equation, asymptotic boundary conditions for approximating the potential at large distances from the gate are proposed. On the basis of calculation results, a controlling parameter is suggested, which allows to determine the localization of electron wave function regardless of insulator thickness and permittivity.

Keywords: FINITE DIFFERENCE METHOD, MIS-STRUCTURE, NANOGATE, SCHRÖDINGER EQUATION, ENERGY LEVEL, NUMERICAL MODELING

1. Introduction

The sensitivity of the electrical, optical, and magnetic properties of semiconductors to doping impurities is widely used to create various semiconductor devices. Reducing the physical size of the devices led to the need for taking into account quantum effects in the design and optimization of modern semiconductor structures [1]. Moreover, the achievements in technology of manufacturing nanoscale structures have made it possible to construct devices with only one impurity atom in the working region [2]. Designing of such devices requires additional fundamental studies devoted to the quantum mechanical modeling of their physical properties.

There are several proposals of using single impurity atoms to physically realize qubits, which can be based on the nuclear spin of a phosphorus impurity in silicon [3], the electron spin of a bound electron [4] or its charge [5]. These proposals stimulated the appearance of a number of papers devoted to modeling the electronic states of a donor near semiconductor surface (see [6-13]). The main attention was paid to the control of the donor electron density with an external electric field when the critical characteristic of the system under study was the critical field [9-10] or the critical potential at the gate [6], which corresponds to the relocation of the wave function of the donor electron into the gate area.

Taking into account all the features of the system (the finite size of the gate, the presence of a dielectric layer of nonzero thickness, the difference between the dielectric permittivities of semiconductor and insulator layers) requires solving the problem for the Laplace equation in a multilayered medium. As a result, it becomes necessary to use numerical methods, in particular, the finite difference method (FDM), which had shown its effectiveness in solving similar problems [14]. Attempts of applying FDM for modeling quantum mechanical effects in nanoscale structures with single donors were made in Refs. [15-16]. However, in these papers, the structures with confining potential of a simple form were considered, that does not require solving the problem for the Laplace equation.

The aim of this paper is to develop an algorithm for the numerical simulation of electronic states in a metal-insulator-semiconductor (MIS) structure with a single donor in the gate region based on sequential solution of the problems for the Laplace equation and the stationary Schrödinger equation. To calculate the gate potential, wave functions, and energy levels, FDM is used. The results of FDM calculations are compared with the results obtained with the finite element method (FEM).

2. Formulation of the problem

We consider a singly charged donor located in semiconductor at a distance z_0 from the semiconductor-insulator interface. An external electric field is created by an infinitely thin disc-shaped gate of diameter d and potential Φ_0 . The insulator layer, separating the gate from the semiconductor, is located in the area $-t_{ox} < z < 0$. The donor and the center of the gate are positioned on the Oz axis.

According to the effective mass approach, the energy E and the electron wave function Ψ for states with zero projection of the orbital angular momentum on the Oz axis are described with the problem for the stationary Schrödinger equation (in cylindrical coordinates):

$$(\hat{T} + \hat{V})\Psi = E\Psi, \quad \rho > 0, \quad z > 0, \quad (1)$$

where \hat{T} is a kinetic energy operator, \hat{V} is a potential energy operator.

In Eq. (1), we use effective Bohr radius as a unit of length

$$a^* = \frac{4\pi\epsilon_0\epsilon_2\hbar^2}{m^*e^2} \quad (2)$$

and effective Rydberg as a unit of energy

$$Ry^* = \frac{\hbar^2}{2m^*(a^*)^2} = \frac{1}{4\pi\epsilon_0\epsilon_1} \frac{e^2}{2a^*}, \quad (3)$$

where m^* is electron effective mass in semiconductor, ϵ_1 is dielectric permittivity of semiconductor. The potential is measured in units of Ry^*/e , respectively.

In Eq. (1), the kinetic energy operator \hat{T} is defined as

$$\hat{T} = -\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial}{\partial \rho} \right) - \frac{\partial^2}{\partial z^2}, \quad (4)$$

The potential energy operator is the sum

$$\hat{V} = \hat{V}_D + \hat{V}_{D'} + \hat{V}_{sim} + \hat{V}_G,$$

where \hat{V}_D is the interaction between the electron and the donor

$$\hat{V}_D = -\frac{2}{\sqrt{(z-z_0)^2 + \rho^2}}, \quad (5)$$

$\hat{V}_{D'}$, \hat{V}_{sim} are the interactions of the electron with the donor image and electron image respectively [12]:

$$\hat{V}_D = -\frac{2Q^*}{\sqrt{(z+z_0)^2 + \rho^2}} + \frac{8\varepsilon_1\varepsilon_2}{(\varepsilon_1 + \varepsilon_2)^2} \frac{\varepsilon_3 - \varepsilon_2}{\varepsilon_3 + \varepsilon_2} \sum_{k=1}^{\infty} \frac{(P^*)^{k-1}}{\sqrt{(z+z_0+2kt_{ox})^2 + \rho^2}}, \quad (6)$$

$$\hat{V}_{sim} = \frac{Q^*}{2z} - \frac{2\varepsilon_1\varepsilon_2}{(\varepsilon_1 + \varepsilon_2)^2} \frac{\varepsilon_3 - \varepsilon_2}{\varepsilon_3 + \varepsilon_2} \sum_{k=1}^{\infty} \frac{(P^*)^{k-1}}{z + kt_{ox}}, \quad (7)$$

where dielectric permittivity of the medium $\varepsilon(\rho, z)$ is

$$\varepsilon(\rho, z) = \begin{cases} \varepsilon_1, & (\rho, z) \in (0, +\infty) \times (0, +\infty) = D_1; \\ \varepsilon_2, & (\rho, z) \in (0, +\infty) \times (-t_{ox}, 0) = D_2; \\ \varepsilon_3, & (\rho, z) \in (0, +\infty) \times (-\infty, -t_{ox}) = D_3; \end{cases} \quad (8)$$

$$Q^* = \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2}; \quad P^* = Q^* \frac{\varepsilon_3 - \varepsilon_2}{\varepsilon_3 + \varepsilon_2}. \quad (9)$$

Operator $\hat{V}_G = -u(\rho, z)$ describes the electron potential energy in external field, where gate potential $u(\rho, z)$ is solution of the following problem:

$$\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \varepsilon \frac{\partial u}{\partial \rho} \right) + \frac{\partial}{\partial z} \left(\varepsilon \frac{\partial u}{\partial z} \right) = 0, \quad \rho > 0, \quad -\infty < z < +\infty, \quad (10)$$

$$\left. \frac{\partial u}{\partial \rho} \right|_{\rho=0} = 0, \quad (11)$$

$$u \rightarrow 0 \quad \text{as} \quad z \rightarrow \pm\infty, \quad \rho > 0, \quad (12)$$

$$u \rightarrow 0 \quad \text{as} \quad \rho \rightarrow +\infty, \quad -\infty < z < +\infty. \quad (13)$$

At the semiconductor boundary, an infinitely high potential barrier is assumed, which allows to set the boundary condition for the wave function in the form

$$\Psi|_{z=0} = 0. \quad (14)$$

For bound states:

$$\Psi \rightarrow 0 \quad \text{as} \quad \rho \rightarrow \infty, \quad z \rightarrow \infty. \quad (15)$$

At points on the axis $\rho=0$ outside the donor location, the wave function must be continuously differentiable, so

$$\left. \frac{\partial \Psi}{\partial \rho} \right|_{\rho=0} = 0, \quad z \neq z_0. \quad (16)$$

At the donor location, condition (16) is not satisfied, since the potential becomes infinite at this point. Using a method described in [11], one can obtain the following condition

$$\left(\frac{\partial \Psi}{\partial \rho} + \Psi \right) \Big|_{\rho=0} = 0, \quad z = z_0. \quad (17)$$

3. Calculation of the gate potential

For numerical calculation of the gate potential, the unbounded domain $\rho > 0$, $-\infty < z < +\infty$, on which the problem is posed, was replaced by a bounded domain $0 < \rho < L_\rho$, $-L_{z3} < z < L_{z1}$. The conditions on the boundary of this domain were set using the assumption that at large distances the gate potential can be approximately assumed to be equal to the potential of the point charge q located in the center of the gate. This potential has been found using Fourier-Bessel transform [18]:

$$v_1(\rho, z) = \frac{q}{\pi \varepsilon_0 (\varepsilon_2 + \varepsilon_3)(\varepsilon_2 + \varepsilon_1)} \sum_{k=0}^{\infty} \frac{(P^*)^k}{\sqrt{(z+t_{ox}(2k+1))^2 + \rho^2}},$$

$$v_2(\rho, z) = \frac{q}{2\pi \varepsilon_0 (\varepsilon_2 + \varepsilon_3)} \left(\sum_{k=0}^{\infty} \frac{(P^*)^k}{\sqrt{(z+t_{ox}(2k+1))^2 + \rho^2}} - \sum_{k=0}^{\infty} \frac{Q^*(P^*)^k}{\sqrt{(z-t_{ox}(2k+1))^2 + \rho^2}} \right),$$

$$v_3(\rho, z) = \frac{q}{4\pi \varepsilon_0 \varepsilon_3} \left(\frac{2\varepsilon_3}{\varepsilon_2 + \varepsilon_3} \frac{1}{\sqrt{(z+t_{ox})^2 + \rho^2}} - \frac{4\varepsilon_2\varepsilon_3}{(\varepsilon_2 + \varepsilon_3)^2} \sum_{k=1}^{\infty} \frac{Q^*(P^*)^{k-1}}{\sqrt{(z-t_{ox}(2k-1))^2 + \rho^2}} \right).$$

After differentiation we get the boundary conditions:

$$\left(\frac{\partial u_1}{\partial z} - \frac{1}{v_1} \frac{\partial v_1}{\partial z} u_1 \right) \Big|_{z=L_{z1}} = 0, \quad \rho > 0, \quad (18)$$

$$\left(\frac{\partial u_3}{\partial z} - \frac{1}{v_3} \frac{\partial v_3}{\partial z} u_3 \right) \Big|_{z=L_{z3}} = 0, \quad \rho > 0, \quad (19)$$

$$\left(\frac{\partial u_k}{\partial \rho} - \frac{1}{v_k} \frac{\partial v_k}{\partial \rho} u_k \right) \Big|_{\rho=L_\rho} = 0, \quad -\infty < z < +\infty, \quad k = 1, 2, 3. \quad (20)$$

Difference scheme for the problem (10) – (11), (18) – (20) was constructed on the grid ω_L , which is defined as follows:

$$\omega_\rho = \left\{ \rho_i = ih_\rho : h_\rho = \frac{L_\rho}{N_\rho}, \quad i = \overline{0, N_\rho} \right\},$$

where h_ρ is a grid step, N_ρ is a number of nodes on ρ direction,

$$\omega_z^{(1)} = \left\{ z_j^{(1)} = jh_z^{(1)} : h_z^{(1)} = \frac{L_{z1}}{N_z^{(1)}}, \quad j = \overline{0, N_z^{(1)}} \right\},$$

$$\omega_z^{(2)} = \left\{ z_j^{(2)} = jh_z^{(2)} - t_{ox} : h_z^{(2)} = \frac{t_{ox}}{N_z^{(2)}}, \quad j = \overline{0, N_z^{(2)} - 1} \right\},$$

$$\omega_z^{(3)} = \left\{ z_j^{(3)} = -L_{z3} + jh_z^{(3)} : h_z^{(3)} = \frac{L_{z3} - t_{ox}}{N_z^{(3)}}, \quad j = \overline{0, N_z^{(3)} - 1} \right\},$$

$h_z^{(k)}$ is a grid step, $N_z^{(k)}$ is a number of nodes on z direction. Then

$$\omega_L = \omega_\rho \times (\omega_z^{(1)} \cup \omega_z^{(2)} \cup \omega_z^{(3)}).$$

The values of the potential in grid nodes are denoted as

$$y_{ij}^{(k)} = u_k(\rho_i, z_j^{(k)}), \quad k = 1, 2, 3.$$

As a result, we get the following difference scheme [14]:

$$\frac{1}{\rho_i} \left(\rho_{i+1/2} y_{i+1/2}^{(k)} \right)_\rho + y_{iz}^{(k)} = 0, \quad k = 1, 2, 3. \quad (21)$$

$$\varepsilon_k \frac{y_{i,1}^{(k)} - y_{i,0}^{(k)}}{h_z^{(k)}} - \varepsilon_{k+1} \frac{y_{i,0}^{(k)} - y_{i, N_z^{(k+1)} - 1}^{(k+1)}}{h_z^{(k+1)}} + \frac{\varepsilon_k h_z^{(k)} + \varepsilon_{k+1} h_z^{(k+1)}}{2} \times \frac{\rho_{i+1/2} (y_{i+1,0}^{(k)} - y_{i,0}^{(k)}) - \rho_{i-1/2} (y_{i,0}^{(k)} - y_{i-1,0}^{(k)})}{\rho_i h_\rho^2} = 0, \quad (22)$$

$$k = 1: \quad i = \overline{1, N_\rho - 1}; \quad k = 2: \quad i = \overline{N_d + 1, N_\rho - 1}.$$

$$\frac{y_{1,j}^{(k)} - y_{0,j}^{(k)}}{h_\rho} + \frac{h_\rho}{4} \frac{y_{0,j+1}^{(k)} - 2y_{0,j}^{(k)} + y_{0,j-1}^{(k)}}{(h_z^{(k)})^2} = 0, \quad (23)$$

$$j = \overline{1, N_z^{(k)} - 1}, \quad k = 1, 2, 3.$$

$$y_{i,0}^{(2)} = \Phi_0, \quad i = \overline{0, N_d}, \quad (24)$$

where $N_d = \lceil d/2h_p \rceil$. Conditions (18) – (20) are approximated with the second order using additional points outside the computational domain and Eqs. (21) – (22).

4. Numerical solving of the Schrödinger equation

As in the case of potential computation, the problem for the Schrödinger equation has been solved on the finite domain $0 < \rho < L_p$, $0 < z < L_{z1}$. Since there is an exponential decay of the wave function at infinity, zero boundary conditions for the wave function were set on the boundary of the computational domain, i.e. the boundary condition (15) has been replaced with the conditions:

$$\Psi|_{z=L_{z1}} = 0, \quad \Psi|_{\rho=L_p} = 0. \quad (25)$$

The solution of the Schrödinger equation has been constructed on a grid:

$$\Omega_S = \omega_\rho \times \omega_z^{(1)}.$$

Denoting the values of the wave function at the grid nodes as

$$w_{ij} = \Psi(\rho_i, z_j^{(1)})$$

we get the following difference scheme:

$$-\frac{1}{\rho_i} \left(\rho_{i+1/2} w_\rho \right)_\rho - w_{zz} + V_{ij} w = E_h w, \quad (26)$$

$$w_{i,0} = 0, \quad i = \overline{0, N_\rho}, \quad (27)$$

$$w_{i, N_z^{(1)}} = 0, \quad i = \overline{0, N_\rho}, \quad (28)$$

$$w_{N_\rho, j} = 0, \quad j = \overline{1, N_z^{(1)} - 1}, \quad (29)$$

where E_h is approximate energy value, $V_{ij} = \hat{V}(\rho_i, z_j^{(1)})$.

To increase the order of approximation of the boundary condition (16), the difference approximation of the Schrödinger equation (1) on the axis $\rho = 0$ is used. As a result, we get

$$w_\rho + \frac{h_p}{4} (w_{zz} - V_{0j} w + E_h w) = 0, \quad j \neq j_0, i = 0, \quad (30)$$

where $(0, j_0)$ is the node corresponding to the donor location. The value of the wave function at the donor location can be found from the second order approximation for the condition (17):

$$3w_{0, j_0} = 4w_{1, j_0} - w_{2, j_0} + 2h_p w_{0, j_0}. \quad (31)$$

5. Error estimation

The error of calculating the energy will be different when the electron is in the gate region and when it is located in the region near the donor. In the first case, both the error in calculating the potential and the error of the solution of the Schrödinger equation affect the accuracy of energy calculation.

To estimate the error in calculating the potential, arising from setting conditions (18) – (20) on the boundaries of computational domain, we consider a test problem in which an infinitely thin disc is in a homogeneous medium or on the boundary of two homogeneous media. In this case, the exact analytic expression for the potential is known [18]. Calculations of the gate potential using FDM have been carried out for three model problems with different conditions on the boundaries of the computational domain. In the first problem, the value of the potential at the boundary is assumed to be zero, in the second problem, the potential on the boundary is exact [18] and, in the third problem, conditions (18) – (20) are set on the boundary. The solutions obtained in all three cases were compared with the exact value of the potential in the integral norm on the domain $0 < \rho < 10a^*$, $-10a^* < z < 10a^*$. Calculations for gate diameter $d = 6a^*$, $L = L_\rho = L_{z1} = L_{z3}$ in range from $10a^*$ to $40a^*$

and grid step $h = h_p = h_z^{(k)} = 0.1$ have shown that the use of the conditions (18) – (20) instead of exact boundary conditions does not increase relative energy error even for small computational domains. On the contrary, when using zero boundary conditions on the boundary of the computational domain, the computational error increases sufficiently: the relative error at $L = 10a^*$ with zero boundary conditions is more than twenty much greater than the corresponding error for the problem with exact boundary conditions.

We consider the case, when the electron is localized on the donor, in the absence of external gate field and image charges. Then, at the donor location, the potential in the Schrödinger equation has a singularity, which can lead to additional errors. In order to verify the effect of condition (17) on the accuracy of the calculations, the dependences of the donor ground state energy on the grid step in the problem with condition (17) and with condition (16) at the donor location were calculated (Fig. 1). As one can see from Fig. 1, the use of the condition (16) at the location of the donor leads to the appearance of additional fluctuations in the error caused by the relative position of the donor location ($\rho = 0$, $z = z_0$) with respect to the grid. Thus, the use of conditions (17) has a significant effect on the accuracy of the computations.

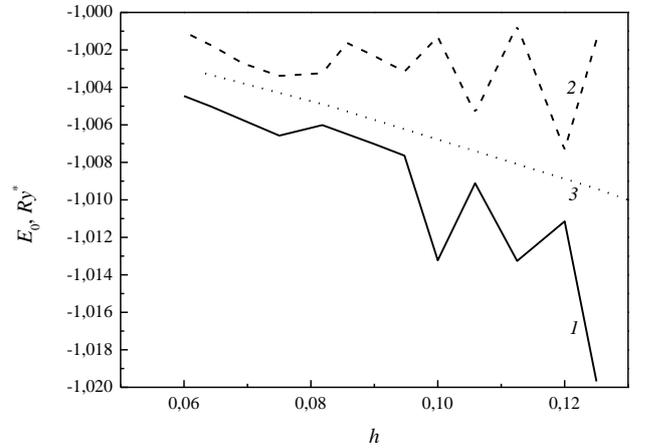


Fig. 1 The effect of non-analyticity of the potential on calculation results of the energies of the ground state (E_0), for the distance from the donor to the semiconductor surface $z_0 = 8a^*$, at zero gate potential and neglecting image charges; h is the grid step. The curves 1, 2 are calculated using FDM and FEM, respectively, with conditions (16) at the donor location, the curve 3 is calculated using FDM with condition (17).

6. Results and discussion

One of the main characteristics of the structure under study is the value of the external electric field at which relocation of electron wave function from the donor to the near-gate region takes place. We denote corresponding critical gate potential as Φ_{0C} . The critical potential depends on a number of parameters of the system: the size of the gate, the position of the donor, the dielectric constant of the media, and the thickness of the dielectric layer.

It had been shown in [19] that the critical field corresponds to a minimum of the difference between the energies of the first excited and ground states ($E_1 - E_0$). Therefore, to determine Φ_{0C} it is sufficient to calculate the energy values of two states, which essentially simplifies the problem.

Dependences of the critical potential on the thickness of the dielectric layer are shown in Fig. 2. As one can see from the figure, the critical potential increases with increasing thickness of the dielectric faster for smaller values of ϵ_2 , e.g., for $t_{ox} = 2a^*$ (≈ 6.3 nm in silicon) $\Phi_{0C} \approx 231$ mV for $\epsilon_2 = 3.8$ and $\Phi_{0C} \approx 95$ mV for $\epsilon_2 = 34.2$. This means that when an insulator with a lower dielectric permittivity is used, the device requires a larger potential at the gate, which additionally increases the probability of dielectric breakdown.

It had been shown in [19] that at zero insulator thickness the redistribution of the ground state wave function depends only on the potential difference between the point of the donor location and semiconductor surface and does not depend on the position of the donor. An analogous dependence also takes place for a nonzero dielectric thickness. We consider the value $\Delta\Phi$ which is the potential difference between the donor and the semiconductor surface:

$$\Delta\Phi = \Phi(0, z_0) - \Phi(0, 0),$$

where

$$\Phi(\rho, z) = \hat{V}_G(\rho, z) + \hat{V}_D(\rho, z) + \hat{V}_{sim}(\rho, z).$$

Correspondingly, we introduce the value of $\Delta\Phi_C$ which is the critical potential difference. The calculations show (Fig. 2) that the value of $\Delta\Phi_C$ is practically independent of the thickness and material of the dielectric. This allows us to use the results of calculations of the critical potential difference for a zero thickness of the dielectric in modeling of structures with an arbitrary thickness of the insulating layer.

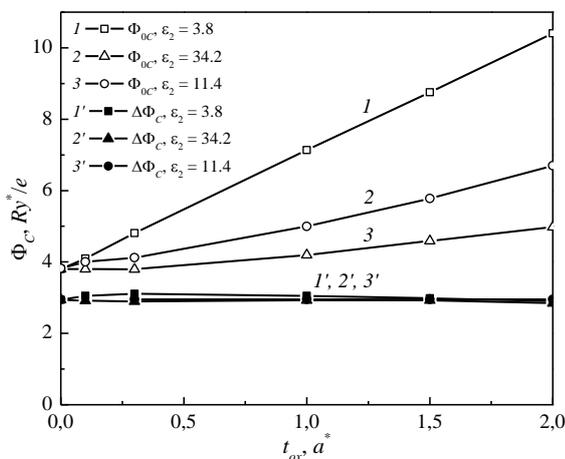


Fig. 2 The dependences of the critical potential (Φ_{0c}) and critical potential difference ($\Delta\Phi_c$) on dielectric thickness for different dielectric constants of the insulating layer; $d = 6a^*$, $z_0 = 8a^*$, $\epsilon_1 = 11.4$, $\epsilon_3 = 1$.

7. Conclusion

Numerical simulation of the electronic structure of a metal-insulator-semiconductor in the presence of a near-surface donor has been carried out. To calculate the gate potential and solve the problem for the stationary Schrödinger equation, a difference scheme has been proposed. A method to approximate the boundary conditions at infinity at calculations of the gate potential has been proposed. It has been found that the use of the proposed boundary conditions makes it possible to significantly reduce errors in calculated potential as compared with the use of zero conditions at the boundaries of calculation domain.

Using the suggested difference schemes, the dependences of the ground and first excited state energies of the donor on the field of disc-shaped gate in a three-layered medium have been obtained. On the basis of these dependences, the critical potential of the gate has been calculated, at which the electron density of the ground states is relocated from the donor to the gate region. It has been found that the critical potential difference between the donor and the semiconductor surface is the controlling parameter when describing the functioning of the device, since it practically does not depend on the thickness and permittivity of the dielectric layer.

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