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CONDENSED MATTER PHYSICS

A Method of Dopant Electron Energy Spectrum Parameterization for Calculation of Single-Electron Nanodevices

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Abstract—Solitary dopants in semiconductors and dielectrics that possess stable electron structures and interesting physical properties may be used as building blocks of quantum computers and sensor systems that operate based on new physical principles. This study proposes a phenomenological method of parameterization for a single-particle energy spectrum of dopant valence electrons in crystalline semiconductors and dielectrics that takes electron–electron interactions into account. It is proposed to take electron–electron interactions in the framework of the outer electron shell model into account. The proposed method is applied to construct the procedure for the determination of the effective dopant outer shell capacity and the method for calculation of the tunneling current in a single-electron device with one or several active dopants–charge centers.

Keywords: single-atom single-electron transistor, dopants.

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INTRODUCTION

Studies of electronic devices with sub-nanometer working elements, "solitary" atoms, result in the development of electronic computer systems with ultrahigh density and performance. Two concepts for the development of single-atom elements have been proposed. One of the concepts is based on the application of molecules in which the working charge center is formed on a chemically separated atom [1]. As a rule, this is a metal atom [1, 2]. The second concept applies separate surface dopants in semiconductor and dielectric crystals [3, 4] and is a continuation of the long-term process of reducing the size of basic elements of traditional semiconductor electronic devices. Dopants in traditional electronic devices are used as passive suppliers of charge carriers, electrons or holes. In single-atom electronic devices dopants are the key functional element [3–5].

The use of solitary dopants as building blocks of solid-state nanoelectronics is attractive due to their stable electron structure, physical properties, and ultrasmall size. The prototypes of such information-processing devices based on new physical principles, such as quantum bits [6–8], quantum gates [9], logic switches [10], and charge pumps [11, 12], have been developed using dopants. Previously, trial experimental implementation of such devices was performed based on classical single-electron devices and cluster molecules [13, 14]. Charge automata based on solitary atomic centers are ideal for the development of rearrangeable computing devices with an ultrahigh information density.

Experimental investigation of a single-electron tunneling transport through solitary dopants is mainly performed using single-electron transistors based on them [3, 8, 15–17]. Such transistors consist of a nanobridge with one or several dopants in its narrowest part, tunneling electrodes, and one or several control electrodes [3, Fig. 1].

The main difficulty in the extremely topical theoretical description from the first principles of electron transport through solitary dopants is a large number of atoms in a cluster of the minimum required size. As an example, for a phosphorus dopant in silicon, the radius of localization of the single-particle wave function of a valence electron is less than 3 nm [18] and the minimum required number of atoms in a model cluster is 10^4. For practically important models the number of atoms in a cluster, as a rule, is even larger, and can reach 10^6 [19]. The large size of the model system requires petaflop-scale computing facilities, which substantially reduces the possibility of regular simulation of atomic functional electronic devices by the wide scientific community. For a number of dopants in model devices on the order of 10 and higher, it is practically impossible to design and describe their evolution from the first principles due to the exponential growth of the number of combinations of quantum and charge states that should be included in the calculation.

In this study, we propose a phenomenological method for the parameterization of a single-particle electron spectrum of dopant valence electrons in semiconductors and dielectrics that drastically reduces the complexity of calculation of electron transport in electronic devices based on solitary dopants. The proposed method is capable of calculating current–voltage and control characteristics and current stability diagrams of such single-electron devices. The application of the proposed method to obtain the capacity characteristics of the dopant as the charge center of a single-electron device is demonstrated.

1. A HYDROGEN-LIKE MODEL IN THE EFFECTIVE MASS APPROXIMATION

The simplest model of the energy spectrum of outer valence electrons of the dopant in crystalline semiconductors such as silicon is the model of a hydrogen-like atom in the "effective mass" approximation [20]. This approximation results in a hydrogen-like [21] energy spectrum of the valence electron. The disadvantage of the effective mass approximation for description of single-electron transfer through solitary dopants is that it is impossible to take multielectron charge and excited states, as well as charging and discharging processes, into account.

The hydrogen-like model in the effective mass approximation can be extended for description of different dopant charge and multielectron quantum states. Before doing this, let us outline some propositions of the model. In the hydrogen-like model, single-particle electron energy levels of dopant valence electrons in a semiconductor in terms of the International System of Units can be written as

$$\varepsilon_n = -\frac{m^* e^4}{2n^2\hbar^2\epsilon^2(4\pi\epsilon_0)^2} = -\frac{m^* e^4}{8h^2n^2\epsilon^2\epsilon_0^2}, \qquad (1)$$

where n is the principal quantum number and m^* is the effective electron mass at the bottom of the semiconductor carrier band [20]. The relative dielectric permittivity ϵ in the denominator of expression (1) is the measure of the dopant Coulomb potential screening by the semiconductor electrons.

The envelopes of the amplitude distribution for single-particle wave functions of the valence electron in the dopant region are similar to the amplitude distributions of the wave functions for an electron in a hydrogen-like atom. The presence of anisotropy in a crystal may result in the reduction of the central symmetry of the effective potential of the dopant and the elimination of random degeneration of single-particle energy levels with respect to the orbital l and magnetic m_l quantum numbers. The carrier band in the hydrogen-like dopant model in semiconductors in the effective mass approximation plays the role of the energy continuum.

Let us write the Bohr orbit radii, the average velocities, and the characteristic frequencies of valence electron motion in dopants for further consideration. The average electron velocity for a state with the principal quantum number n is

$$r_n = \frac{\epsilon\epsilon_0 n^2 h^2}{\pi m^* e^2}, \quad v_n = \frac{e^2}{2\epsilon\epsilon_0 hn} = \frac{G_0}{2\epsilon\epsilon_0 n}, \quad \nu_n = \frac{m^* e^4}{4\epsilon^2\epsilon_0^2 n^3 h^3}, \qquad (2)$$

where G_0 is the conductance quantum. The radius of the nth Bohr orbit in a hydrogen-like atom, for example, an arsenic atom in silicon and $n = 1$ is $r_1 \approx 2.2$ nm.

2. A MODEL OF THE ELECTRON-ENERGY SPECTRUM WITH ACCOUNT FOR THE ELECTRON–ELECTRON INTERACTION

A specific feature of current stability diagrams of single-atom single-electron devices is the presence of a series of so-called Coulomb diamond patterns with rather constant tunneling current values [3, 15–17]. In such devices, in the course of tunneling transport several electrons can be localized under the action of external control fields by increasing the effective depth of the potential-energy well in the dopant region. Since the dopant has several weakly bound electrons it is necessary to take their Coulomb interaction into account, which results in the appearance of Coulomb diamond patterns in the current stability diagrams of single-electron single-atom devices.

Let us determine the localized single-particle states of valence electrons in dopants similar to usual miltielectron atoms [21, 22]; each of such states is determined by the set of four quantum numbers $p = (n, l, m_l, m_s)$. Localized Wannier functions [20, 23] can be considered as an appropriate model for such states. Here, these states are determined phenomenologically based on the analysis of existing experimental current stability diagrams of single-electron dopant-based transistors [3, 15–17]. The principal quantum number n in such states determines the size of the wave function localization region for the corresponding single-particle state; it can be equal to $n \approx 1, 2, 3$ .... The orbital quantum number l determines the angular distribution of the electron density around the dopant center. The quantum number m_l determines the orientation of the spatial electron-density distribution. Let us define the set of introduced single-particle electron states localized in the dopant with the quantum number n as a shell, the set of states with the same values of (n, l) as a subshell, and the set of states with the same values of (n, L, m_s) as a half-subshell. Similar definitions for free atoms are well known in atomic physics [21, 22].

The presence of the dopant violates the translational symmetry of the semiconductor. At the same time, central symmetry of the dopant core is violated by the crystalline lattice. For this reason, while considering single-particle electron wave functions one may speak of the orbital mechanical momentum of the dopant valence electrons or the electron momentum in the semiconductor carrier band.

The key assumption of the proposed phenomenological model is the equality of the single-particle electron energy in one half-subshell of the dopant (n, l, m_s). In the case of weakened requirements for the precision of electron-energy determination, the difference in the electron energy for the two halves of the same atomic subshell or different subshells of the same shell can be neglected.

The experimental data on measurement of the ionization potentials for free atoms [24] indicate that the outer half of the subshell for a free atom with the quantum numbers (n, l, m_s) can be considered from the point of view of the model of an ideal sphere with the certain ideal radius $R_{n'}$ [25, 26]. This approach was used in this study for the description of dopant shells in semiconductors. The energy of the dopant electron shells in a semiconductor formally can be calculated based on their averaged radius and the electron interaction model on an ideally conducting sphere [25, 27]. Let us write the electrostatic electron interaction energy for such an ideal sphere with the radius R_{nlm_s} [25, 27],

$$E_{ee,n'}(N_{nlm_s}) = \frac{N_{nlm_s}(N_{nlm_s}-1)e^2}{8\pi\epsilon\epsilon_0 R_{nlm_s}}, \quad (3)$$

where N_{nlm_s} is the number of electrons in the half-subshell (nlm_s). The factor ($N_{nlm_s} - 1$) considers the absence of electron–electron interaction in the case of one electron in the subshell [25].

The energy of attraction of N_{nlm_s} electrons to the dopant core for the chosen half-subshell can be written as

$$U_{Ze,nlm_s}(N_{nlm_s}) = -\frac{N_{nlm_s}Z^*_{nlm_s}e^2}{4\pi\epsilon\epsilon_0 R_{nlm_s}}, \quad (4)$$

where $Z^*_{nlm_s}$ is the effective charge of the dopant core for the half-subshell (n, l, m_s), which includes the electron charge of all lower electron shells and the charge of the nucleus.

The kinetic energy of N_{nlm_s} electrons in the half-subshell can be determined as

$$T_{nlm_s}(N_{nlm_s}) = \frac{N_{nlm_s}\hbar^2 n^2}{2m^* R^2_{nlm_s}}. \quad (5)$$

The total energy of the dopant half-subshell with N electrons and the principal quantum number n is

$$E_{nlm_s}(N_{nlm_s}) = N_{nlm_s} \times\left(\frac{\hbar^2 n^2}{2m^* R^2_{nlm_s}} - \frac{(Z^*_{nlm_s} - (N_{nlm_s}-1)/2)e^2}{4\pi\epsilon\epsilon_0 R_{nlm_s}}\right). \quad (6)$$

The effective radius of the half-subshell can be determined by minimization of its total energy (6) with respect to R_{nlm_s},

$$R_{nlm_s}(N_{nlm_s}) = \frac{4\pi\epsilon\epsilon_0\hbar^2 n^2}{e^2 m^*(Z^*_{nlm_s} - (N_{nlm_s}-1)/2)}. \quad (7)$$

Let us estimate $Z^*_{nlm_s}$ for the arsenic dopant in silicon. The second half of its 4p subshell is external and incompletely filled in the ground state. It contains just one electron. The effective charge of its core can be estimated using the energy of the excited single-particle state of the arsenic atom in silicon equal to 0.048 eV [20] as $Z^*_{4p} \approx 5.3$. If this half-subshell is completely filled, $(N_{4p} - 1)/2 = 1$. This estimate shows that, as a rule, $Z^*_{nlm_s} \gg (N_{nlm_s} - 1)$, which is determined by the non-ideal character of the dopant core screening by inner shell electrons. Expression (7) can be considered as an improved expression for the Bohr radius in a dopant (2). Expression (7) allows one to define the notion of the effective dopant shell capacity [28, 29],

$$C_{nlm_s}(N_{nlm_s}) = \frac{(4\pi\epsilon\epsilon_0)^2\hbar^2 n^2}{e^2 m^*(Z^*_{nlm_s} - (N_{nlm_s}-1)/2)}. \quad (8)$$

The effective capacities of two half-subshells of one subshell differ slightly. The difference of the capacities can be estimated as

$$\Delta C \sim \frac{e^2}{E_{ls}}, \quad (9)$$

where E_{ls} is the characteristic energy of spin-orbital interaction for the chosen subshell.

Expression for the effective radius of the electron shell in the dopant (7) can be used to obtain the expression for the total energy of the half-subshell,

$$E_{nlm_s}(N_{nlm_s}) = -\frac{e^2 m^*(Z^*_{nlm_s} - (N_{nlm_s}-1)/2)^2}{2(4\pi\epsilon\epsilon_0)^2\hbar^2 n^2}. \quad (10)$$

The average electron velocity in the considered half-subshell is written as

$$v_{nlm_s}(N_{nlm_s}) = \frac{e^2(Z^*_{nlm_s} - (N_{nlm_s}-1)/2)}{4\epsilon\epsilon_0 hn}. \quad (11)$$

The characteristic motion frequency in the dopant for the chosen half-subshell is

$$\nu_{nlm_s}(N_{nlm_s}) = \frac{m^* e^4 (Z^*_{nlm_s} - (N_{nlm_s} - 1)/2)^2}{(4\pi\epsilon\epsilon_0)^2 n^3 \hbar^3}. \quad (12)$$

Expressions (11) and (12) are extensions to the multielectron case of the corresponding Bohr formulas.

The electrostatic energy of the N_{nlm_s} electron in the half-subshell can be calculated in the proposed model based on the following expression:

$$\varepsilon_{nlm_s}(N_{nlm_s}) = \frac{e^4 m^* \left(Z^{*2} + \left(\frac{3}{4} N_{nlm_s} - 2Z^*_{nlm_s} - 1\right)(N_{nlm_s} - 1)\right)}{2(4\pi\epsilon\epsilon_0)^2 \hbar^2 n^2}. \quad (13)$$

The presence of several electrons in the same half-subshell and their equivalence explain the reason of existence of several blockade Coulomb diamond patterns with the same Coulomb blockade in the current diagrams of single-atom single-electron transistors, while the Bohr model of the dopant predicts monotonic reduction of Coulomb blockade diamond patterns with an increasing principal quantum number.

3. A METHOD FOR THE CALCULATION OF THE TUNNELING CURRENT THROUGH THE DOPANT

In earlier experimental studies [3, 15–17] the measured electric resistance of the single-electron dopant-based transistor bridge was 10^5–10^8 Ω. Since the quantum unit of resistance is 25.8 Ω and the electron transport through dopants in these studies was performed presumably through several single-particle energy levels, the tunneling barrier transparency between the dopants and the tunneling electrodes can be estimated as 2×10^{-1}–2×10^{-4}. For such a tunneling barrier transparency and a not very high bias voltage, single-particle electron states of the dopant are weakly bound with single-particle states of other dopants and electrodes, which corresponds to the single-electron mode of tunneling transport [27, 33].

The tunneling rate between dopants and dopants and electrodes can be estimated using the expression for the characteristic frequency of valence electron motion in the electron shell of the dopant (12),

$$\Gamma_{nlm_s}(N_{nlm_s}) \approx \nu_{nlm_s}(N_{nlm_s}) \tau_{nlm_s}(N_{nlm_s}), \quad (14)$$

where $\tau_{nlm_s}(N_{nlm_s})$ is the transparency coefficient for the effective tunneling barrier between a pair of dopants or between a dopant and an electrode for the corresponding valence electron energy $\varepsilon_{nlm_s}(N_{nlm_s})$. The height of the effective potential barrier is determined in the "effective mass" approximation as the difference between the carrier band bottom and valence electron energy in the dopant (13). The width of effective tunneling barrier is determined by the distance between neighboring dopants or between a solitary dopant and a tunneling electrode. The tunneling coupling between the dopants or between a solitary dopant and a tunneling electrode results in broadening of single-particle electron energy levels in dopants by $\hbar\Gamma_{nlm_s}(N_{nlm_s})$. The size of the electron localization region increases with increasing n and l; therefore, the effective capacity and electron tunneling rate for the corresponding subshells increase.

In a single-atom single-electron transistor the energy of electrostatic interaction between the dopant that play the role of an active charge center and a metal tunneling electrode can be described using effective mutual electric capacities $C^{\mathrm{L}}_{nlm_s}$ and $C^{\mathrm{R}}_{nlm_s}$ [30]. Let us determine the bias voltage division factor for a single-electron transistor at the point of the dopant with respect to the tunneling electrodes as

$$\eta_{nlm_s}(N_{nlm_s}) = \frac{C^{\mathrm{L}}_{nlm_s}(N_{nlm_s})}{C^{\mathrm{L}}_{nlm_s}(N_{nlm_s}) + C^{\mathrm{R}}_{nlm_s}(N_{nlm_s})}. \quad (15)$$

It can be assumed with high precision that the bias voltage division factor is independent of the quantum number of the dopant subshell,

$$\eta_n \approx \eta. \quad (16)$$

Let us write the electrostatic energy of a partially filled half-subshell as

$$U_{nlm_s}(N_{nlm_s}) = \frac{N_{nlm_s}(N_{nlm_s} - 1)e^2}{2C^{\Sigma}_{nlm_s}(N_{nlm_s})} - N_{nlm_s} e(\varphi_{\mathrm{g}} + \varphi_{\mathrm{t}}). \quad (17)$$

where

$$C^{\Sigma}_{nlm_s}(N_{nlm_s}) = C_{nlm_s}(N_{nlm_s}) + C^{\mathrm{L}}_{nlm_s}(N_{nlm_s}) + C^{\mathrm{R}}_{nlm_s}(N_{nlm_s}); \quad (18)$$

φ_{g} is the electric potential created at the point of the dopant by the control electrodes; φ_{t} is the electric potential created by the parasitic charge traps, "passive" charge centers, which can be formed by various crystalline lattice defects and other dopants that do not take part in the electron transport. The presence of such traps complicates the analysis of the characteristics of single-electron dopant-based devices, since these traps can be spontaneously charged and discharged with a certain small probability. For this reason, the exact determination of φ_{t} is rather difficult. In experiments on the creation of single-atom single-electron devices, the potentials φ_{g} and φ_{t}, similar to the potentials of tunneling electrodes, are determined with respect to the lower conducting layer of the substrate which is usually neutral. These potentials at the position of the active atomic charge center should be understood as the potential drops that define the additional shift of the dopant energy levels.

The electron subshells of the dopant with the energy lower than the valence shell remain unexcited and are not taken into account in single-electron transport. The total charge state of the dopant N is determined as the difference of the total number of electrons localized at the dopant in the charged state and the number of localized electrons in the neutral dopant. The charge state $N = 0$ corresponds to the electrically neutral dopant. The total electrostatic energy of the dopant can be written as the sum of electrostatic energies of all subshells,

$$U(N) = \sum_{\{nlm_s\}} \left[\frac{N_{nlm_s}(N_{nlm_s} - 1)e^2}{C^{\Sigma}_{nlm_s}} - N_{nlm_s} e(\varphi_g + \varphi_t) \right]. \quad (19)$$

Let us obtain the expression for calculation of the tunneling current in single-electron devices in which the effective charge centers are dopants in the approximation of the weak tunneling coupling. Let us assume that the width of single-particle energy levels of the dopant valence electrons determined by the tunneling coupling is small compared to the average distance between them. Let us also assume that the width of these levels is much smaller than thermal fluctuations,

$$kT \gg h(\Gamma^{L}_{N,p} + \Gamma^{R}_{N,p}), \quad (20)$$

where $p = (n, l, m_l, m_s)$ and is much smaller the characteristic Coulomb energy of a solitary dopant [27, 33],

$$E_C \gg h(\Gamma^{L}_{N,p} + \Gamma^{R}_{N,p}), \quad (21)$$

We also neglect resonance tunneling through the dopant, assuming that it makes a much smaller contribution to the tunneling current than single-electron tunneling.

Let us write the expression for the electron tunneling probability in unit time to $w^{+}_{n,N,p}$ and from $w^{-}_{n,N,p}$ of the single-particle energy level p of a solitary dopant [27, 31],

$$\begin{aligned} w^{+}_{N,p} &= w^{L,+}_{N,p} + w^{R,+}_{N,p} = \Gamma^{L}_{N,p} f^{+,L}_{N,p} + \Gamma^{R}_{N,p} f^{+,R}_{N,p} \\ w^{-}_{N,p} &= w^{L,-}_{N,p} + w^{R,-}_{N,p} = \Gamma^{L}_{N,p}(1 - f^{-,L}_{N,p}) + \Gamma^{R}_{N,p}(1 - f^{-,R}_{N,p}), \end{aligned} \quad (22)$$

where $f^{\pm,L(R)}_{N,p}$ is the Fermi–Dirac distribution calculated for the corresponding energies of single-particle levels in the left and right electrodes for electron arrival "+" and departure "–" from the dopant [27, 31]. The tunneling rate in expression (22) can be calculated based on expression (14) or Fermi's golden rule [27] and Bardin's approximation [32]. In calculation of probabilities (22), it is necessary to consider the energy conservation for the electron tunneling to the final (from the initial) single-particle state $p = (n, l, m_l, m_s)$ in the dopant subshell in the charge state N_{nlm_s} from the initial (into the final) state in the left (right) electrode to the energy level $\varepsilon_{\pm,L(R)}$,

$$\begin{aligned} \varepsilon^{\pm,L(R)} &= \varepsilon_{N,p} \pm U(N_{nlm_s} \pm 1) \\ &\mp U(N_{nlm_s}) - \eta^{L(R)} eV + e(\varphi_g + \varphi_t), \end{aligned} \quad (23)$$

where $\eta^{L} = \eta$, $\eta^{R} = \eta - 1$.

It is necessary to use the density matrix technique for description of the evolution of the quantum states of the dopant. In the case of weak tunneling coupling, using the secular and Markov approximations, one can use the description of the system using the probability distribution function $\rho(\{n_p\}, t)$ for the populations n_p of the single-particle states $p = (n, l, m_l, m_s)$ and the system of kinetic equations [27, 31] in which the tunneling probabilities are determined by expressions of form (22). If the system of kinetic equations for the probability distribution function $\rho(\{n_p\}, t)$ is solved, the tunneling current through a single-atom single-electron transistor can be calculated. For this purpose, it is necessary to calculate the current through one of the two tunnel junctions of the transistor, since in the stationary mode the currents through the left and right transitions are equal,

$$\begin{aligned} I = I^{L} = I^{R} = -e \sum_{p=1}^{\infty} \sum_{\{n_j\}} \rho(\{n_i\}, t) \{ &\delta_{n_p,0} w^{L,+}_{n,N,p}(V, \varphi_g, \varphi_t) \\ &- \delta_{n_p,1} w^{L,-}_{n,N,p}(V, \varphi_g, \varphi_t) \}, \end{aligned} \quad (24)$$

where n_p are the populations of single-particle electron energy levels in the dopant.

4. THE CONDUCTIVITY OF THE SINGLE-PARTICLE ELECTRON ENERGY LEVEL

For a low bias voltage V, electron transport through the dopant is possible through one single-particle electron level with the index p. In this case, the sum in expression (24) includes just one term. Using the approximate expression for the conductivity of a single energy level in the linear response approximation in the limit $V \to 0$ obtained earlier in [31], we write the conductivity of the single-atom transistor as

$$G \approx \frac{e^2}{4k_B T} \frac{\Gamma^{L}_{N,p} \Gamma^{R}_{N,p}}{\Gamma^{L}_{N,p} + \Gamma^{R}_{N,p}} \frac{1}{\cosh^2(\varepsilon^{\pm,L(R)}/2k_B T)}. \quad (25)$$

Usually, experiments are performed close to the symmetric single-atom single-electron transistor, $\eta \approx 0.5$ and $\Gamma^{L}_{N,p} \approx \Gamma^{R}_{N,p} \approx \Gamma_{N,p}$. In experimentally used transistors [3, 15–17], the measurements were mainly performed at helium ($T = 4$ K) and lower temperatures. The values of $\varepsilon^{\pm,L(R)}$ correspond to the position of single-particle dopant energy levels with respect to the carrier band of the crystal. As an example, for silicon and superficial donors, these energy values are ~10 meV, which allows one to replace hyperbolic cosine by unity

with good precision in expression (25). Using the maximum tunneling conductivity measured experimentally at the Coulomb diamond pattern boundary, let us write a simpler expression for estimation of the effective tunneling barrier transparency,

$$G_{\max} = \max\left\{\frac{\partial I}{\partial V}\right\} = \frac{e^2}{4k_BT}\Gamma_{N,p}. \quad (26)$$

The final expression for the tunneling barrier transparency coefficient is obtained by substituting the expression for $\Gamma_{N,p} \sim \nu_{nlm_s}(N_{nlm_s})\tau_p$, where the frequency $\nu_{n,N}$ is determined by expression (12). As a result, we have

$$\tau_{N,p} = \frac{G_{\max}}{G_0}\frac{k_BT}{\pi \mathrm{Ry}}\frac{m_e}{m^*}\frac{\epsilon^2 n^3}{(Z^*_{nlm_s} - (N_{nlm_s}-1)/2)^2}. \quad (27)$$

Using the approximate expression for the transparency of a rectangular tunneling barrier and assuming that the effective height of the potential barrier between the dopant and the tunneling electrode is determined by the energy difference between the bottom of the semiconductor crystal carrier band and the single-particle energy level of the dopant, the width of the effective tunneling barrier can be estimated as

$$\mathcal{W} \approx -\frac{\hbar \ln(\tau_{N,p})}{2\sqrt{2m^*\varepsilon_{N,p}}}. \quad (28)$$

Expression (28) gives an estimate for the distance between solitary dopants and between dopants and tunneling electrodes.

5. DETERMINATION OF THE EFFECTIVE CAPACITY OF THE OUTER DOPANT SHELL

The phenomenological model of the dopant electron shells presented above allows one to determine their effective radius and effective capacity by processing the data of experimental measurements of the current stability diagrams for a single-atom single-electron transistor. The energy conservation law (23) can be used for determination of the capacity parameters for atomic shells of the dopant active charge center. In the limit of low temperature $T \to 0$ Coulomb diamond patterns in the current stability diagram have a clear inner microstructure and edges. The boundaries of each diamond are determined by the probabilities of including and excluding single-particle states of a particular electron shell into the tunneling electron transport through the dopant.

Using expression (17), we can write the variation of electrostatic energy for electron tunneling to the half-subshell (nlm_s) as

$$U(N_{nlm_s}+1) - U(N_{nlm_s}) = \frac{N_{nlm_s}e^2}{C^{\Sigma}_{nlm_s}} - e(\varphi_g + \varphi_t). \quad (29)$$

It follows from expressions for the transition probability (22) that the probability of tunneling to the energy level p of the shell with the principal quantum number n and the charge state N is nonzero, $w^+_{n,N,p} > 0$ if

$$\varepsilon_{N,p} \le \eta^{\mathrm{L(R)}}eV - \frac{N_{nlm_s}e^2}{C^{\Sigma}_{nlm_s}} + e(\varphi_g + \varphi_t). \quad (30)$$

The probability of electron tunneling from the single-particle energy level p of the dopant in the charge state N is nonzero, $w^-_{n,N,p} > 0$, if the following condition is satisfied:

$$\varepsilon_{N,p} \ge \eta^{\mathrm{L(R)}}eV - \frac{(N_{nlm_s}-1)e^2}{C^{\Sigma}_{nlm_s}} + e(\varphi_g + \varphi_t). \quad (31)$$

If the conditions $w^+_{n,N,p} > 0$ and $w^-_{n,N,p} > 0$ are not satisfied for any charge state N and single-particle energy level p of the active dopant center, then the total current through the transistor is zero, $I = 0$.

Expressions (30) and (31) determine the positions of Coulomb diamond patterns in the current stability diagram. The transition on such diagram from the region with zero tunneling current $I = 0$ to the region with nonzero current $I \neq 0$ is connected with opening of one of the single-particle energy levels of the dopant for tunneling transport.

Equalities (30) and (31) and the data on the structure of blockade diamonds in the current stability diagram allow one to estimate the capacity parameters of the transistor dopant center e^2/C_Σ and C_Σ [27, 33]. For this purpose, let us determine the mutual capacity of the transistor active dopant charge center and the control electrode. This problem is complicated by the presence of parasitic charge traps. If the charge states of these traps do not change with small variation of the bias voltage V and the control voltage V_g, then the potential φ_g can be determined using linear approximation of the Coulomb diamond boundary in the current stability diagram. It can be seen using conditions (30) and (31) that the Coulomb blockade diamond boundary can be written as

$$\varphi_g = \alpha_g V_g = \eta^{\mathrm{L(R)}}V + \mathrm{const}. \quad (32)$$

The choice of η^{L} and η^{R} in expression (32) is determined by which side of the Coulomb diamond is chosen for determination of the capacity coefficient of the control electrode α_g. Finally, we obtain

$$\alpha_g = \eta\left.\frac{dV}{dV_g}\right|_{\mathrm{rb}} \quad \text{or} \quad \alpha_g = (\eta - 1)\left.\frac{dV}{dV_g}\right|_{\mathrm{lb}}, \quad (33)$$

for the capacity coefficient of the control electrode, where the indices "lb" and "rb" denote the left and right boundaries of the current diamond, respectively.

Using expression (33), we find the bias voltage division factor,

$$\eta = \left.\frac{dV}{dV_G}\right|_{\text{lb}} \Big/ \left(\left.\frac{dV}{dV_G}\right|_{\text{lb}} - \left.\frac{dV}{dV_G}\right|_{\text{rb}}\right). \quad (34)$$

We can apply expressions (30) and (31) for determination of the values of e^2/C_Σ and C_Σ. Using the two neighboring vertices of the current triangles that correspond to single-particle electron energy levels $\varepsilon_{N,p'}$ and $\varepsilon_{N,p''}$ from the same half-subshell and two charge states N' and $N'' = N' \pm 1$ of the dopant, and assuming that the surrounding charge traps do not change their charge state, and therefore, do not change the electric potential at the point of the active dopant with varying voltage at the control electrode from one vertex to the other, and applying (30) and (31) for $V = 0$, we obtain the following expression for estimation of the characteristic Coulomb energy of the working charge center of the transistor:

$$\frac{e^2}{C^{\Sigma}_{nlm_s}} \approx \frac{\varepsilon_{N',p'} - \varepsilon_{N'',p''} - e\alpha_g(V_g' - V_g'')}{N'' - N'}. \quad (35)$$

CONCLUSIONS

A phenomenological method for parameterization of single-particle energy spectrum of dopant valence electrons in crystalline semiconductors and dielectrics was proposed; this method is the development of the hydrogen-like model in the effective mass approximation for superficial dopants in semiconductors. The presence of electron–electron interaction and electron shells are taken into account in the proposed method. The electron shell parameters can be determined from experimental data or based on the calculation from the first principles.

The technique for determination of effective capacity of dopant valence electrons was presented; this is extremely important for analysis of experimental results aimed at development of single-atom single-electron devices.

The method for calculation of the tunneling current in a system of one or several dopants and tunneling electrodes was proposed based on the above method for parameterization of single-particle energy spectrum. Use of the data from the calculation of the dopant electron structure in semiconductors and dielectrics to obtain the electron-shell parameters is proposed for further development of this method. The description of single-particle dopant electron states in semiconductor and dielectric crystals is complicated by anisotropy. The proposed shell model can be altered to take anisotropy into account by replacing spherical shells with ellipsoidal ones, if necessary.

The proposed parameterization of the energy spectrum of valence electrons in dopants makes it possible to use simulation of electron transport in practically interesting single-electron nanodevices consisting of one or several active dopants, for example, dopant-based charge automata.

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