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Steps on current-voltage characteristics of a silicon quantum dot covered by natural oxide

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Considering a double-barrier structure formed by a silicon quantum dot covered by natural oxide with two metallic terminals, we derive simple conditions for a step-like voltage-current curve. Due to standard chemical properties, doping phosphorus atoms located in a certain domain of the dot form geometrically parallel current channels. The height of the current step typically equals to $(1.2\,\mathrm{pA})N$, where $N = 0, 1, 2, 3\ldots$ is the number of doping atoms inside the domain, and only negligibly depends on the actual position of the dopants. The found conditions are feasible in experimentally available structures.

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The fabrication of Si nanostructures became possible through recently developed new technologies [1, 2]. Individual silicon quantum dots (SQD) reported in [2] are spherical Si particles with diameters d in the range $5 - 12$ nm covered by a $1 - 2$ nm-thick natural SiO_2 film. Metallic current terminals made from degenerately doped Si are defined lithographically to touch each individual dot from above and from below.

To ensure metallic electrodes the donor concentration n should be $n \geq n_{\mathrm{Mott}}$, where $n_{\mathrm{Mott}} = 7.3 \times 10^{17}\,\mathrm{cm}^{-3}$. The critical concentration n_{Mott} is defined by the Mott criterion [3], introducing the transition to a metallic type of conductivity in a semiconductor at:

$$a_B (n_{\mathrm{Mott}})^{1/3} = 0.27 \qquad (1)$$

where a_B is the Bohr radius of an electron bound to a donor inside the Si crystal, in the case of phosphorus-donors $a_B = 3$ nm [4].

As for the doping of the dot, the situation concerning a Mott transition in that small dots is much less trivial than the one described by Eq. (1). Let us consider dots with diameters $d = 10$ nm formed from n-doped Si with $n = n_{\mathrm{Mott}}$ as an illustrative example. Then each dot contains in average one donor. Note that we will consider degenerately n^+-doped electrodes with $n \gg n_{\mathrm{Mott}}$ which ensures metallic conduction up to the borders of the dot.

Real fabrication technology [2] provides a wafer with hundreds of SQDs on it with current leads towards each individual SQD. Dots in average have the same value of mean dopant concentration n, which is determined by the parent material of bulk silicon the dots are formed from. However, on the level of each individual SQD we will always have exactly *integer* number of doping atoms. If, as in the example above, the average number of dopants $\overline{N_{\mathrm{tot}}} = 1$ the actual number of donors in the dot can have values $N_{\mathrm{tot}} = 0, 1, 2, 3, \ldots$, with values larger than these very unlikely.

Our objective is to illustrate, that SQDs from the same wafer fall into several distinct sets of approximately the same conductance. The typical value of conductance for each set is nearly completely determined by the number N of donors present in a certain part of a SQD so that N labels each set of SQDs.

Summarizing the above, we need for a quantization of the conduction through a dot with N donors the following conditions:

- Size d of the dot comparable with Bohr radius: $2 < d/a_B < 5$.
- Average doping n of the dot $n \leq d^{-3}$, leading to a mean number of dopants $\overline{N_{\mathrm{tot}}} \leq 1$, so that $N_{\mathrm{tot}} = 0, 1, 2$ are the most probable configurations of an individual SQD.
- Doping of the electrodes $n_{el} \gg n_{\mathrm{Mott}}$, so that current leads are perfectly metallic.
- Dot covered by an oxide layer thick enough to suppress ballistic transport through the dot.

In fact all these condition can be simultaneously satisfied for SQD fabricated with the method mentioned above [2].

Model system. We use a simple model of a cubic SQD with $d > 2a_B$ (we will use $d = 10$ nm for

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estimates), covered with an oxide layer with thickness $\delta = 2\,\mathrm{nm}$, height [4] $B = 3.15\,\mathrm{eV}$ and contacted with current terminals from left and from right. The x-axis is oriented from left to right along the current flow, as shown in Fig.1.

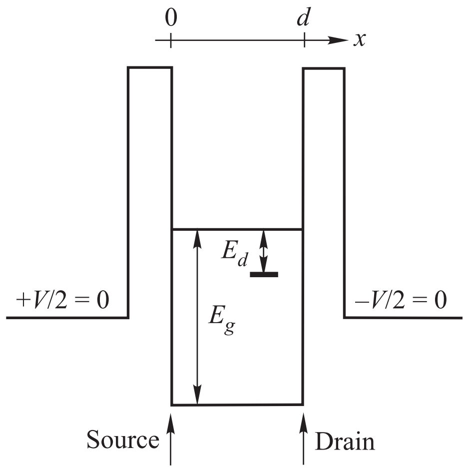

Fig.1. Potential profile of the dot covered by an oxide layer at $V = 0$. A donor is marked with a short bar

A tunneling current is injected into the dot via the oxide barrier from the top (source at $x = 0$) and leaves the dot at the bottom (drain at $x = d$). Due to the presence of the oxide barriers this current is non-ballistic and non-thermal. We assume that the high potential barriers associated with the oxide layers are not much affected by the voltage and the tunneling charges. We concentrate on what happens between these effective source and drain (Fig.2), as in [5].

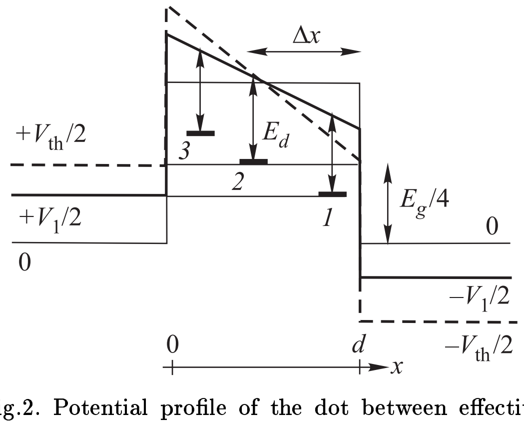

Fig.2. Potential profile of the dot between effective source and drain biased with $V_{\mathrm{eff}} = V_1$ (thick solid line) and $V_{\mathrm{eff}} = V_{\mathrm{th}}$ (dashed line)

In the case when the dot can be regarded as an insulating system it is reasonable to assume that the applied voltage equally drops over the potential barriers and the dots. For simplicity we neglect the difference of the dielectric constants of the oxide barriers and the dot. In this approximation we can introduce an effective voltage $V_{\mathrm{eff}} = V(d - 2\delta)/d = 0.6\ V$ describing the part of the total transport voltage V applied between effective source and drain which drops across the dot itself.

In this rude approximation we neglect the effect of spatial quantization upon values on the ionization energy, the conductivity gap and material parameters of silicon.

Dot without donors. At $V_{\mathrm{eff}} = 0$ the Fermi level inside the dot is situated in the middle of the gap, i.e. $E_g/2$ bellow the conduction band edge ($E_g = 1.14\,\mathrm{eV}$ at 300 K).

As V_{eff} grows, the bottom of the (still empty) conduction band bends down accordingly. When the conduction band in the dot close to the drain aligns with the Fermi level of the emitter we expect a drastic increase in the tunneling current. This threshold V_{th} voltage (Fig.2) for V_{eff} is given by $V_{\mathrm{th}} = E_g/2e$, regardless of the number N_{tot} of dopants in the dot (as long as the dot is not yet metallic, of course). In the following we therefore limit our studies to voltages

$$|V_{\mathrm{eff}}| \le V_{\mathrm{th}} = E_g/2e = 0.57\,\mathrm{V}. \tag{2}$$

In this voltage range we have a d-thick barrier (formed by the dot) with always finite height between effective source and drain. The intrinsic concentration of electrons and holes at 300 K is $1.4 \cdot 10^{10}\,\mathrm{cm}^{-3}$. Even at this high temperature the probability to have at least one intrinsic electron in a dot with size $d = 10\,\mathrm{nm}$ is only $1.4 \cdot 10^{-8}$. So we would expect virtually no current in this mode. This is confirmed by direct electrical tests [2] of SQD with the required properties.

Single-donor channel. Let us now consider one single donor in the dot located at x with ionization energy [4] $E_d = 0.045\,\mathrm{eV}$ (for P as a donor).

At zero temperature current is due to resonant tunneling via non-ionized donor (as in [6] for example). Differential conductance $g(\varepsilon)$ for the states with energy ε is

$$g(\varepsilon) = \frac{4e^2}{\pi\hbar} \frac{\Gamma_\ell \Gamma_r}{(\varepsilon - \varepsilon_d)^2 + (\Gamma_\ell + \Gamma_r)^2}, \tag{3}$$

where $\Gamma_{\ell,r}$ is linewidth of $1s$ state of electron bound to the donor due to coherent mixing with conduction states to the left (right) of the left (right) tunnel barrier.

Oxide barriers (with height $B = 3.15\,\mathrm{eV}$ and width $\delta = 2\,\mathrm{nm}$) give dominant contribution to $\Gamma_{\ell,r}$ compared to contribution of the body of the dot (with typical height $< E_g/2 = 0.57\,\mathrm{eV}$ and width $< d = 10\,\mathrm{nm}$). So, we can approximate $\Gamma_{\ell,r}$ with linewidth Γ for the case of an impurity localized at distance δ inside rectangular one-dimensional tunnel burrier [6] of height B:

$$\Gamma_\ell = \Gamma_r = \Gamma = \frac{2p_F\kappa}{p_F^2+\kappa^2} B \frac{\exp(-2\kappa\delta)}{\kappa\delta} = 2.5\cdot 10^{-9}\,\mathrm{eV}, \tag{4}$$

where m is (true, not effective) electron mass, $\kappa = (2mB)^{1/2}/\hbar$, and $p_F = (2mE_F)^{1/2}/\hbar = \left(3\pi^2 n_{\rm el}\right)^{1/3}$ is Fermi wave number in the contact electrodes. The numerical estimate in (4) is given for the electrodes doped up to $n_{\rm el} = 10^{21}\,\mathrm{cm}^{-3}$ as in [2].

Within approximation (4) point $\varepsilon = \varepsilon_d$ brings function $g(\varepsilon)$ given by (3) to a sharp maximum $g(\varepsilon_d) = e^2/\pi\hbar$ of width $\Gamma \ll V_{\rm th}$.

From Fig.2 it is clear that resonant energy $\varepsilon_d = E_g/2 - xV_{\rm eff}/2ed - E_d$. This means that as soon as effective Fermi level $eV_{\rm eff}/2$ reaches a certain threshold $eV_1/2$, tunnel current J flowing through the structure acquires a step-like increase of

$$J_1 = \frac{1}{e}\int\limits_{-eV/2}^{eV/2} g(\varepsilon)d\varepsilon = \frac{g(\varepsilon_d)2\pi\Gamma}{e} = \frac{2e\Gamma}{\hbar} = 1.2\,\mathrm{pA}, \tag{5}$$

If the impurity is located near the drain, i.e. $d - a_B < x < d$ (as donor *1* in Fig.2), then threshold V_1 for the effective voltage $V_{\rm eff}$ is given by

$$V_1 = E_g/2e - E_d/e = 0.525\,\mathrm{V}. \tag{6}$$

In contrast, for an impurity located at distances $\Delta x > 2dE_d/E_g$ from the drain (i.e. further away than the threshold case of donor *2* in Fig.2), no additional current channel via a single impurity can be opened at low enough voltages defined in (2) where virtually no background current is present. In the present case this value $\Delta x = 0.8\,\mathrm{nm}$, which returns us to the above criterion: only impurities located in the immediate vicinity (defined within the accuracy a_B) of the drain contribute to the single-impurity channel.

This shows that in first approximation the conductance of this channel does not depend on x. As shown above, a single-impurity channel already only selects impurities located within a very narrow range of x close to the drain.

Two-, three-, multi-donor channel. The above consideration shows, that due to the bend of the bottom of conduction band following the transport voltage, there is no chance to notice current flowing through a sequential chain of impurities (such as donors *1* and *3* in Fig.2), connecting source and drain. The contribution of such a chain will be totally masked by the current flowing directly via the conduction band. The only way for multiple impurities to manifest themselves in quantized conductance is to form multiple *geometrically parallel* singe-impurity channels situated close enough to the drain as considered above.

Therefore, if $N > 1$ impurities fall into the thin layer near the drain to approximately the same x coordinate as that of donor *1* in Fig.2 (within the Bohr radius), we will see a switching-on of an N-fold channel with current

$$J_N = NJ_1 = N2e\Gamma/\hbar = (1.2\ \mathrm{pA})N \tag{7}$$

at the same threshold voltage $V_{\rm eff} = V_1 = 0.525$ V as for a single-donor channel (Fig.3).

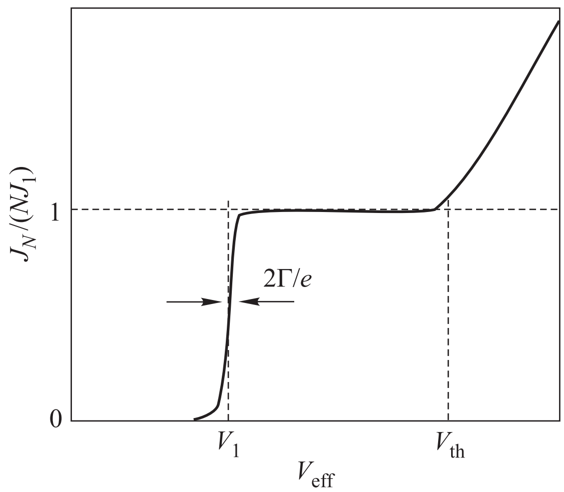

Fig.3. Current-voltage characteristic of a model system (not to scale)

All the above considerations are only valid as long as the dot itself can be regarded as an insulating system. As the number of donors in a SQD grows, the dot becomes a metallic particle, and the conduction band edge in the dot aligns with the Fermi level of the electrodes. In a very simple estimate we define this transition to a metal when the total volume of $N_{\rm tot}$ donors with an individual volume of $(4\pi/3)a_B^3$ exceeds the volume of the dot. This is an exaggerated version of the Mott criterion (1) which holds not only in bulk, but in a small structure, too. For the analyzed example from above this gives $N_{\rm tot} = 8$ as a limiting value. The practically interesting set $0, 1, 2, 3, \ldots$ for both $N_{\rm tot}$ and N considered above is still far bellow this limit.

Quite a number of other mechanisms of electron transport might take place in this system. Surprisingly, even taking into account such other mechanisms [7] does not change much the main idea of the present paper.

In small dots with diameter $d < 2a_B = 6\,\mathrm{nm}$ the domain with N active dopants extends to the whole dot, and thus $N = N_{\mathrm{tot}}$. In large dots with diameter $d > 2a_B = 6\,\mathrm{nm}$ the domain with active dopants is less than the dot itself and is localized near the drain. Hence the position of the domain, number N and value J_N all can be different for the current flowing in different directions. Really, when sign of applied voltage changes, the source and the drain change places.

In a certain sense the discrete increase of dot's conductivity which follow the increase of the dopants number could be regarded as a *mesoscopic analog of the Mott transition* between insulating and conducting states of the system.

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