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Electrical conductivity of silicon quantum nanowires

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We suggest a new theory for the description of electrical conductivity of semiconductor quantum nanowires. We take into account that oscillations of quantum nanowires lead to their self-similar deformation, and because of interaction between nanowires they form fractal clusters. Electrical potential of these structures is described via nonlinear fractal measures. We conclude that current-voltage characteristics of quantum nanowires contain hysteresis loops with oscillations. This fact corresponds to existence of negative differential resistance due to multi barrier tunneling effect in the described fractal structures.Our theoretical results have been confirmed by results of corresponding specific experimental study of nanoscale wire-like structures in silicon.

Key words: silicon, quantum nanowire, tunneling effect, hysteresis, nonlinear fractal.
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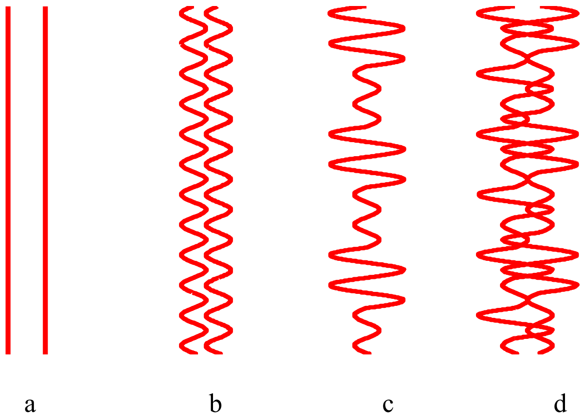
1 Introduction

Silicon quantum nanowires (SiNWs) have been attracting considerable attention due to various application of nanowires in nanoelectronics, optoelectronics, sensor devices [1-6]. Microphotographs of SiNWs show sets of separated groups of nanowires. Each group contains several interacting nanowires. It can be explained by overlapping of wave functions of the nanowires. So, we can consider such structures as quantum nanowires.

At the present time singularities of electrical conductivity of quantum nanowires considered in theoretical and experimental studies on the base of Landauer's theory [7, 8]. In a one-dimensional regular quantum wire density of states is inversely proportional to speed of electrons. In case of a single electron, electrical conductivity is a constant value expressed via the Planck constant and electron charge. This result follows from the Heisenberg's uncertainty principle also. Structure of quantum wires can be irregular,so, in this case we must take into account not only external potential between electrodes ("reservoirs") but value of potential caused by internal heterogeneous distribution of electrons. According to [7] this potential is called the "scattering potential", but its physical nature hasn't been described. In order to define values of current we must integrate relations including probability density function of these potentials, and use different approximations of these relations: uneven (for example, via the Heaviside step function) and wave-like (classical). But irregular alternation of probability density function of distribution of electrons on energies is possible only near absolute zero. quasi-classical description can be used in case of motion of quantum particles with relatively big impulses in a potential field with small gradients. In our case these conditions are improbable. Effective mass and impulse of an electron in a semiconductor are substantially less than effective mass and impulse of a quasi-free electron in a metal. Nano-sized semiconductors have fractal structure with sharp variations of potential barriers. Semiconductor nanofilms can be characterized by existence of hierarchy of similar structures with fractal dimensions in range of spatial scales from 10 to 10^3 nanometers [9]. Results of recent studies show that electrical conductivity of semiconductor nanostructures is a non-monotone function, andcurrent-voltage characteristics of such structures contain areas with negative differential resistance and hysteresis cycle. So, the aim of our work is to construct a simple nonlinear theory for the description of electrical conductivity of semiconductor quantum nanowires accounting values of potential of internal fractal structures, and to compare the theoretical results with our experimental study of SiNWs.

2 Model of clustering of quantum nanowires and theory of electrical conductivity

Let us consider an ensemble of semiconductor nanowires. Diameter L of a nanowire is about sum of size of several atomic layers and the de Broglie wavelength λ of an electron. As usual, L is about 50 nanometers [1-6]. Nanowires can be considered as nonlinear objects because their properties depend on processes in the nanowires. Thermal fluctuations and non-uniform electric potential of boundary aggregation of molecules (ions) disturb shape of nanowires. The simplest and universal algorithm of nonlinear evolution of initially harmonic perturbations (leading to dynamical chaos) is doubling of period. Amplitude of perturbations decreases during a spatial period. The next period characterized by increasing of the amplitude. As a result, wave functions of two nanowires overlap each other (Figure 1). Next stages of evolution of the perturbations can lead to chaotic distribution of electrons in a space with cellular fractal structure. So, a fractal harness consisting of two wires can be formed in a direction perpendicular to the wire. A similar harness formed in three-dimensional space consists of three wires ($\pi^d/_d = \pi \approx 3$). Correlations of third and higher order are possible also, but probability of this case is low.



a) single wire, b) harmonic perturbations of wires,
c) doubling of perturbation period of the single wire,
d) forming of a harness with cellular structure consisting of two wires in the first cycle of doubling of perturbation period with phase shift.

Figure 1 – Model of clustering of quantum nanowires

So, we can take into account a possibility for realization of more complex cycles of overlapping of wave functions and existence of impurity atoms. This approach let to obtain an image of harness of nanowires with fractal structure similar to experimental data. Below we shall describe more complex evolution of perturbations than doubling of period.

3 Quantum electrical conductivity of a fractal nanowire

Let us consider a quantum wire with ideal contacts without scattering. Voltage between the contacts is U An electron moves inside of fractal cluster formed of quantum wires under the influence of potential $V(U)$. We shall describe the potential below. Current corresponding to a single electron is equal to product of density of states $g(E)$ in the energy range eV on speed of electrons $\upsilon(E)$ and value of elementary charge e:

$$I = g(E)\upsilon(E)e. \tag{1}$$

Let us define density of states for unit of length equal to distance between contacts via differential of impulse dP and the Planck constant h [7] as

$$g(E) = \frac{2dP(E)}{h} = \frac{2dE}{h\, {}^{dE}\!/_{dP}} = \frac{2}{h}\frac{dE}{\upsilon(E)} = \frac{2eV(U)}{h\upsilon(E)}. \tag{2}$$

Coefficient “2” in the Eq. 2 is necessary for taking into account the possibility of motion of electrons in two (opposite) directions. From Eqs. (1) and (2) we have

$$I = G_0 V(U),\ G_0 = \frac{2e^2}{h},\ \frac{1}{G_0} = R_0 = 12906\,\Omega, \tag{3}$$

where G_0 is fundamental conductivity. Value $G_0/2$ is called the quantum unit of conductivity, and $2R_0$ is quantum resistance. If conducting channel passes N electrons and M modes (one standing half-wave), the result follows from the Landauer’s theory can be written as [7]

$$G = G_0 \sum_{n,m}^{M} T_{n,m} N_{n,m}(E), \tag{4}$$

where $T_{n,m}$ is probability of transmissions from m – th mode of one contact to n – th mode of another contact, $N_{n,m}(E)$ is number of electrons on the level corresponding to full energy E of the m – th and n – th modes. For quantum nanowires $M = 1$ and by use of delta-symbol we have

$$\sum_{n,m}^{M} T_{n,m} N_{n,m}(E) = \delta_{n,m} N_{n,m}(E) = N(E). \quad (5)$$

Let us designate relative values of potential $V(U)$ between clusters with numbers i and j as $V_{ij}(U)$, and probability of this relation as P_{ij}. Fractal clusters are located chaotically, so, value of total potential difference can be defined as potential difference between ends of a circuit consisting of K elements.

By analogy with Eq. (5) at $k = 1$ we have

$$\sum_{i,j}^{K} P_{ij} V_{ij}(U) = \delta_{ij} V_{ij}(U) = V(U). \quad (6)$$

Function $V = V(U)$ called the "scattering potential" (according to [7]) in our case can be considered as a nonlinear fractal measure characterizing metastable states. We consider measure as a measurable additive value. As usual, fractal measure can be defined by scale of measurement δ depending on structure of an object. Structure of nanowires changes according to applied voltage U. Therefore, we must choose scales of measurement corresponding to variations of the measure as

$$\delta_U = \left|1 - \frac{V(U)}{U}\right|, \ \delta_V = \left|1 - \frac{U}{V(U)}\right|. \quad (7)$$

Indexes at δ describe the determining variables. Values δ_U and δ_V can be used for the description of metastable threshold phenomena at $U \sim V$. We can describe the scattering potential via Eq. (7) and definition of nonlinear fractal measure leading to the Hausdorff's formula for fractal dimension by the following way:

$$V(U,\delta_U) = V_0\left(\left|1 - \left|\frac{V(U)}{U}\right|\right|\right)^{-\gamma},$$

$$V(U,\delta_V) = V_0\left(\left|1 - \left|\frac{U}{V(U)}\right|\right|\right)^{-\gamma}, \quad (8)$$

$$\gamma = D - d,$$

where D is fractal dimension of the set of values $V(U)$, d is its topological dimension. Eqs. (8) contain only difference between D and d. Therefore, these relations can be used for the description as geometrical as physical spaces. At $\gamma = 0$ we have $V(U) = V_0$ which is a non-fractal (for regular structures) value of $V(U)$.

We can use $V_0 = E_g$ as a rank value, where E_g is band-gap energy of silicon measured in electron-volts. Choice of $V_0 = E_g$ as a rank value can be explained by the fact that this value characterizes interruption of energy on boundaries of structures (Brillouin zones).

Equation (3) defines value of current in a regular (non-fractal) nanowire. Fractality is an integral characteristic. Electrical conductivity is a differential, local characteristic. Therefore, we use an expression for fractal measure for resistance $R(U)$ instead of R_0. In this case from Eqs. (3)-(8) we have the following system of equations for the description of current in a nanowire:

$$I(U) = \frac{V(U)}{R(U)}, \quad (9)$$

$$V(U) = V_0\left(\left|1 - \left|\frac{V(U)}{U}\right|\right|\right)^{-\gamma}, \quad (10)$$

$$R(U) = R_\lambda\left(\left|1 - \left|\frac{U}{I(U)R(U) - V_0}\right|\right|\right)^{-\gamma}. \quad (11)$$

Values of current influence on properties of nanowires, so, we can use difference between current and $V_0/R(U)$ as a determining variable in Eq. (11). Resistance R_λ depends on length of a fractal nanowire considered as fractal measure, and can be expressed via relative scale of length λ/L as

$$R_{\lambda} = R_0 \left(\frac{\lambda}{L} \right)^{-(D-d)}, \tag{12}$$

where λ is the de Broglie wavelength, L is size of an area including nanowires, $2R_0$ is quantum resistance. D is fractal dimension of an area ($D > 3$) including considered fractal wires ($d = 1$), therefore, $2 < (D - d) < 3$.

Fine structure of quantum nanowires can be described via relation for second generation of hierarchical structure of cluster potential as

$$V(U) = V_0 \left| 1 - \frac{V(U)}{V_0 \left| 1 - \dfrac{V(U)}{U} \right|^{-\gamma}} \right|^{-\gamma}. \tag{13}$$

4 Results of numerical analyses and experiment

All parameters of our theory have a certain physical meaning. So, we can choose values of these parameters according to a considered problem.

At first, let us define $V(U, \delta_U)$ according to Eq. (8). In order to choose value of the parameter $\gamma = D - d$ we take into account that generally d isn't equal to the greatest integer part of D. For a one-dimensional curve $V(U)$ d – 1,1 < D < 2 therefore, $0 < \gamma < 1$. $V_0 = E_g = 1.12$ eV for silicon. Curve $V(U, \delta_U)$ is non-monotone, there are several peaks at $U \geq V_0$. Amplitude of the peaks growths with increasing of γ (Figure 2).

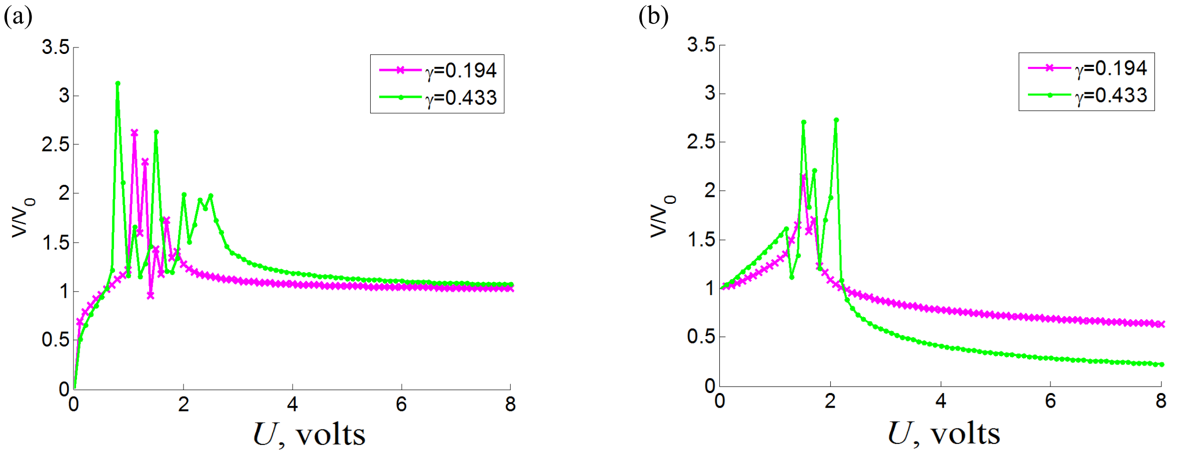


Figure 2 – Curves $V(U, \delta_U)$ and $V(U, \delta_V)$ for different γ according to Eqs. (8) at $V_0 = 1.12$ V.

$V_0 = E_g$ is maximal value of negative potential of an electron localizing in a cluster. So, values of modulus $V(U, \delta_U)$ should be considered as values of potential effecting on electron. Sign of the potential equals to sign of U (determining variable for relative scale of measurement). For correct choosing of determining variable of the required potential $V(U, \delta_U)$ at $U = 0$ we must take into account value of eigen potential barrier of the cluster $V(U = 0, \delta U) = V_0$.

Dependence $I = I(U)$ described by Eqs. (9)-(11) has sharp oscillations at $U \approx V_0$ and saturates at $U > V_0$ (Figure 3). Curves $I(U)$ are intersects each other at different γ_1 and γ_2. In the cross points one metastable state with parameter of fractal dimension γ_1 transfers to another metastable state characterized by γ_2. Hysteresis curves (universal physical phenomena in mediums with metastable states) are located between the cross points of curves $I(U)$.

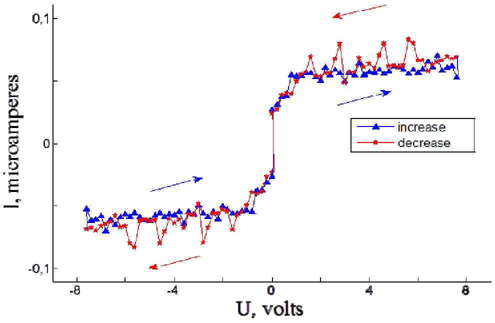


Figure 3 – Theoretical current-voltage characteristics of quantum nanowires for different γ at $R_\lambda = 28$ MΩ, $V_0 = 1.12$ B, γ: ▲ – 0.095, ★ – 0.128.

Electrical conductivity of a nanowire *G(U)* = *1/R(U)* calculated by use of Eqs. (9)-(11) increases due to influence of external voltage *U* and described by corresponding growth of γ (Figure 4).

Main theoretical results obtained on the base of the stated above theory have been checked by our specific experiment. SiNWs were fabricated by well-known metal-induced chemical etching [5, 11, 12] according to the scheme shown in Figure 5. The method consists of three stages: deposition of solution of $AgNO_3$:HF as catalyst, chemical etching in H_2O_2:HF during 40 minutes, and removal of remains of metals in HNO_3. We used p-type crystalline silicon doped by boron as a substrate. Thickness of films is 300 mkm, crystallographic direction is (100), surface resistance of the substrate is 10 Ω·mm^2.

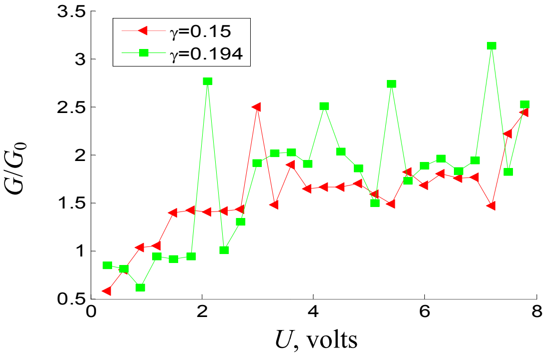


Figure 4 – Variation of electrical conductivity of a nanowire vs voltage for different γ.

$$G_0 = \frac{1}{R_0} = \frac{1}{28\,M\Omega} = 4.3478 \cdot 10^{-8}\ S.$$

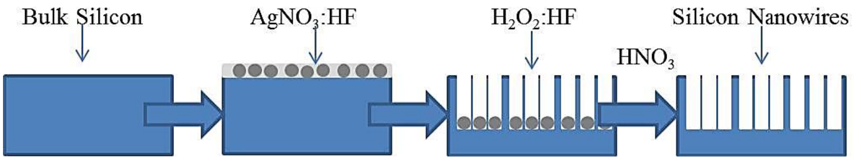


Figure 5 – Scheme for metal-induced chemical etching

We studied the fabricated films by atomic-force microscope. Results of this study are shown in Figure 6.

Results of the study show that length of the considered wire-like structures is about 1÷5 micrometers (Figure 6a), and diameter is 25÷200 nanometers (Figure 6b). Figure 6c shows that distance between sets of wire-like structures is about 100÷500 nanometers.

In case of vertical nanowires metal electrodes must be connected to two ends of SiNWs in order to measure value of resistance of the nanowires. Metal electrode must be closely connected to the end of nanowire. For this aim we used of surface-contact structures shown in Figure 7. Experimental dependence *I(U)* (Figure 8) is a hysteresis curve with a set of loops.

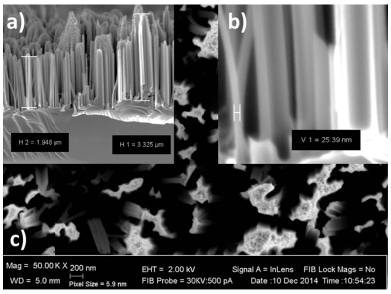


Figure 6 – AFM microscopic image of SiNWs.
a) lateral view (medium zoom), b) lateral view on separate nanowires (maximal zoom), c) top view.

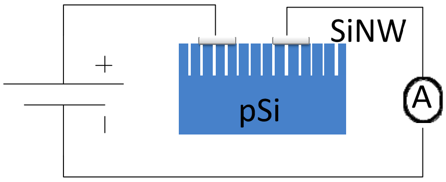


Figure 7 – Scheme of electrical contacts of the sensor with vertical SiNWs (vertical contact).

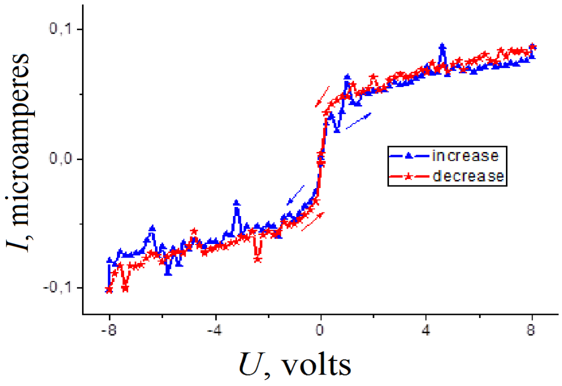


Figure 8 – Experimental current-voltage characteristics of SiNWs

A similar dependence *I(U)* follows from Eqs. (9)-(13) (Figure 9). According to Eq. (10) at the absence of external field value of potential of cluster affecting on electrons *V(U) – 0*, therefore, $I|_{U=0}$ – 0. Growth of *U* leads to increasing of *V(U)*, resistance of quantum nanowire decreases (according to Eq. (11)), and *I(U)* increases sharply. At further growth of *U* value of *V(U)* tends to V_0, and current saturation is observed. But at *U* – V_0 function *V(U)* became a nonlinear fractal measure, and *I(U)* pulses. It indicates to existence of multi-barrier tunneling effect leading to negative differential resistance at *V(U)* – V_0.

In non-fractal crystal ($\gamma = 0$) $V = V_0|_{R_0}$ at $0 < U < V_0$, and inclination of *I(U)* doesn't change. It's equivalent to using of $V(U, \delta_V)$ in Eq. (8), i.e. we use *V(U)* – V_0. as a main variable (instead of *U*). Therefore, we have $I = V(U) – V_0/R_0$ at $U = 0$. For more precision description of the dependence *I(U)* we can take into account second generation of fractal hierarchy of potential according to Eq. (13). In this case we can notice an insignificant growth of inclination of the curve *I(U)* relative to abscissa axis in comparison with this dependence shown in Figure 3 at the same *γ*.

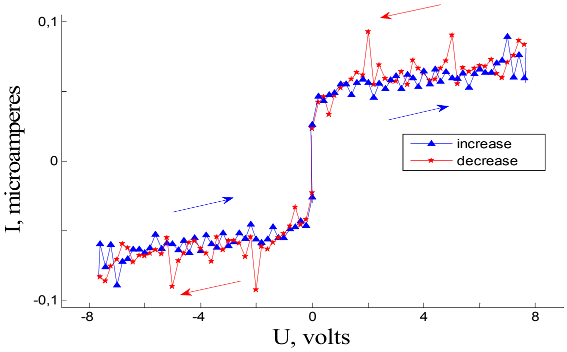


Figure 9 – Theoretical current-voltage characteristics of SiNWs with taking into account their fractal hierarchy according to Eqs. (9)-(13) for different γ at $R_\lambda = 28\,\mathrm{M\Omega}$, $V_0 = 1.12\,\mathrm{eV}$, γ: ▲ – 0.095, ● – 0.128.

Hysteresis in current-voltage characteristics have been observed in different experiments. For example, electrical conductivity of Au/pentacene/Si-nanowire arrays has been studied in [4]. Existence of negative differential resistance has been registered in recent works, for example, in current-voltage characteristics of nanowires and nanobelts *ZnO* [13, 14]. But quantitative descriptions of singularities of these effects haven't been suggested in the works.We suppose that taking into account the fractal structure of nonlinear quantum nanowires let us to obtain the new results.

Thus, our theoretical results obtained via Eqs. (9)-(13) and experimental data adequately describe main physical singularities of electrical conductivity of semiconductor quantum nanowires.

5 Conclusions

Electrical conductivity of nanoscale wire-like structures depends on value of internal potential of fractal clusters. Scattering potential of the clusters can be considered as a nonlinear measure defining by value of external voltage.

Fractality of geometry of wire-like formations leads to appearance of multi-barrier effects in nanoscale wires grown on surfaces of homogeneous films (silicon). Because of this fact the current-voltage characteristic of SiNWs has areas with negative differential resistance and hysteresis loops. Previously such effects have been observed in silicon compounds and heterostructures, but in the present work we describe this phenomena in pure silicon. Results of the present work can be used for perfection of electronic memory schemes, devices of nanoelectronics and optoelectronics.

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