Sn nanothreads in GaAs: experiment and simulation

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ABSTRACT

The gated GaAs structures like the field-effect transistor with the array of the Sn nanothreads.was fabricated via delta-doping of vicinal GaAs surface by Sn atoms with a subsequent regrowth. That results in the formation of the chains of Sn atoms at the terrace edges. Two device models.were developed. The quantum model accounts for the quantization of the electron energy spectrum in the self-consistent two-dimensional electric potential, herewith the electron density distribution in nanothread arrays for different gate voltages is calculated. The classical model ignores the quantization and electrons are distributed in space according to 3D density of states and Fermi-Dirac statistics. It turned out that qualitatively both models demonstrate similar behavior, nevertheless, the classical one is in better quantitative agreement with experimental data. Plausibly, the quantization could be ignored because Sn atoms are randomly placed along the thread axis. The terahertz hot-electron bolometers (HEBs) could be based on the structure under consideration.

Keywords: nanothreads, vicinal surface, conduction anisotropy, hot-electron bolometer

1. INTRODUCTION

We consider an array of Sn-nanothreads (NTs) inserted in GaAs layer [1, 2]. In the novel structure there are the side contacts (the source and drain) and the gate electrode as schematically shown in Fig. 1. Such structures can be fabricated using vicinal GaAs substrates with the surface inclined with respect to the (100) direction by the angle of 0.3-0.1 degree. After growing a thin GaAs layer (with the thickness 0.5 - 1 _m) on such a substrate, the surface constitutes an array of the terraces with one monolayer height (0.28 nm) and the spacing between the terraces about of 50 nm. The delta-doping of this surface by Sn atoms results in the formation of the chains of these atoms (i.e., NTs) at the terrace edges (Fig. 1, below).

On overgrowing the obtained structure, one acquires the array of the NTs inserted in the GaAs substrate. The free electrons accumulated around the Sn NTs form conducting channels along the NTs. The average electron density can be controlled by the gate voltage *Vg*. Varying the latter, one can obtain isolated electron channels. In this case, the conductivity along these channels and perpendicular to them can be markedly different. The anisotropy of the lateral conductivity of the structures under consideration without a gate was observed recently [1, 2].

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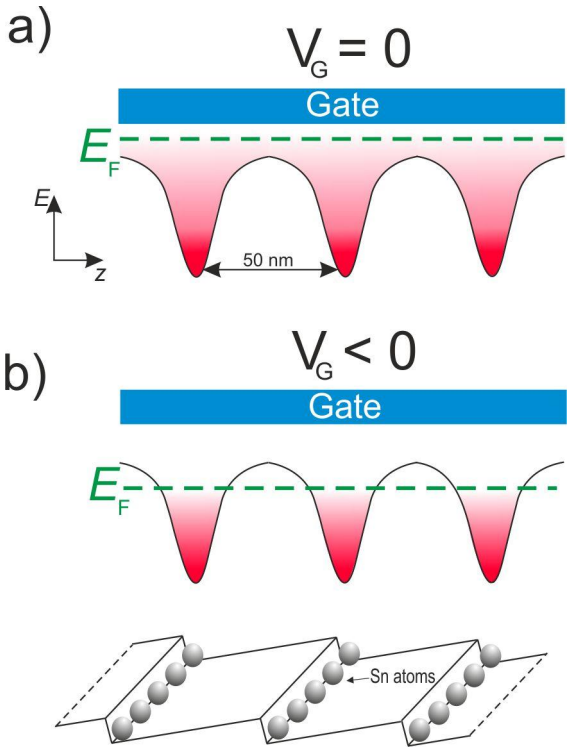

Figure 1. Fermi level controlled by the gate voltage: for zero gate voltage (without a gate) (a) and for negative gate voltage (b). Sn atoms collected in kinks of vicinal surface (below).

2. EQUATIONS OF THE CLASSICAL MODEL

Figure 1 schematically patterns the energy band structure where the position of the Fermi-level is controlled by the gate voltage. The source-drain current is determined by the electrons propagating in the nanothread array plane perpendicular to the nanothreads. This current is created by the electrons with the energies exceeding the height of the potential barriers between nanothreads. The electron spatial and energy distributions are found using the two-dimensional Poisson equation for the self-consistent electric potential φ , formed by the charges of the electrons in the localized states in the channels around each nanothread and in the delocalized states above the barriers. The equation of the model under consideration can be presented as:

$$\frac{\partial^2\varphi}{\partial x^2}+\frac{\partial^2\varphi}{\partial y^2}=\frac{4\pi|e|}{\varepsilon}\left[n(x,y)-q\delta(x)\delta(y)\right]. \qquad (1)$$

Here $e = |e|$ is the electron charge, $\delta(x)$ and $\delta(y)$ are Dirac delta-functions, ε is a permittivity, q is a charge of a nanothread core per unit length, provided $q = \_S_nL$, where $\_S_n$ is the Sn surface density (in cm^{-2}) and L is the distance between the nanothreads, therefore, q is the main factor of the problem, which is determined by the structure parameters. On introducing the dimensionless variables: $\Phi = |e|\varphi/T$, $\xi = x/l_D$, $\zeta = y/l_D$, $\tilde{n}(\xi,\zeta) = n(x,z)/n_T$, $Q = q/(n_T l_D^2)$ where $l_D = \sqrt{\varepsilon T/4\pi e^2 n_T}$ is the Debye screening length for the characteristic electron density $n_T = \frac{(2mT)^{3/2}}{3\pi^2\hbar^3}$, where m is the electron effective mass in GaAs, T is the electron temperature in the energy units (i.e., actually k_BT), and $\hbar$ is the reduced Planck constant, one obtains

$$\frac{\partial^2\Phi}{\partial\xi^2}+\frac{\partial^2\Phi}{\partial\zeta^2}=\left[\tilde{n}(\xi,\zeta)-Q\delta(\xi)\delta(\zeta)\right]. \tag{2}$$

The normalized density of free electrons around the nanothread n and the normalized linear density of charged Sn impurities are given by a Fermi integral

$$\tilde{n}(\xi,\zeta)=\int_0^\infty \frac{d\varepsilon\sqrt{\varepsilon}}{\exp[\varepsilon-\mu-\Phi(\xi,\varsigma)]+1} \quad . \tag{3}$$

The condition of the neutrality of the system on the whole at gate voltage equal to zero (ungated structure) gives a value of the Fermi energy which will be further sustained at zero point to describe equilibrium with source/drain contacts (in other words, all energies will be referenced to the Fermi level)

$$\int_{-l/2}^{l/2} d\xi \int_{-w_s}^{w_g} d\varsigma n(\xi,\varsigma)=Q+\frac{U_{gl}}{w_g} \tag{4}$$

where $l = L/l_D$ is the dimensionless period of the structure (spacing between the nanothreads) and $w_s = W_s/l_D$, and $w_g = W_g=l_D$ are the sizes in the vertical direction (these quantities are also parameters). In the ungated structure $w_s = w_g = w >> l$.

$$\frac{\partial\Phi}{\partial\xi}\Big|_{\xi=\pm l/2}=\pm\varepsilon=\pm\frac{eVl_D}{TL} \tag{5}$$

(periodic boundary condition) and the quantity w should be chosen sufficiently large, so that the result would be weakly dependent on w.

$$\Phi\Big|_{\varsigma=w_g}=U_g\,. \quad \frac{\partial\Phi}{\partial\varsigma}\Big|_{\varsigma=-w_s}=0 \tag{6}$$

where U and U_g are the normalized (by T/e) source-drain voltage per period and gate voltage, respectively. The quantity w should be chosen sufficiently large, so that the result would be virtually independent of w_s.

3. RESULTS OF SIMULATION

The calculated spatial dependence of electron potential energy in the source-drain direction for different gate voltage at room temperature T=300K are depicted in Fig. 2. For negative gate voltage the Fermi level immerges into the potential well. The structure parameters are chosen to be as follows: the mean doping level is Σ_{Sn}=7.5 10^{12}cm^{-2}, the spacing between nanothreads is equal to 50 nm, the same is the distance from threads to the gate. The Gaussian distribution of Sn impurities around the nanothread axis was taken into consideration instead of idealized delta-functions in Equ. 1

$$D(x,y)=\frac{1}{\pi\cdot a^2}\exp(-\frac{x^2+y^2}{a^2})\,. \tag{7}$$

In Fig. 2 and hereafter (but Fig. 6) the Gaussian parameter a is equal to 1 nm, that is, it covers approximately two adjacent lattice nodes. The spreading is a reason why the potential depth in nanothreads is finite.

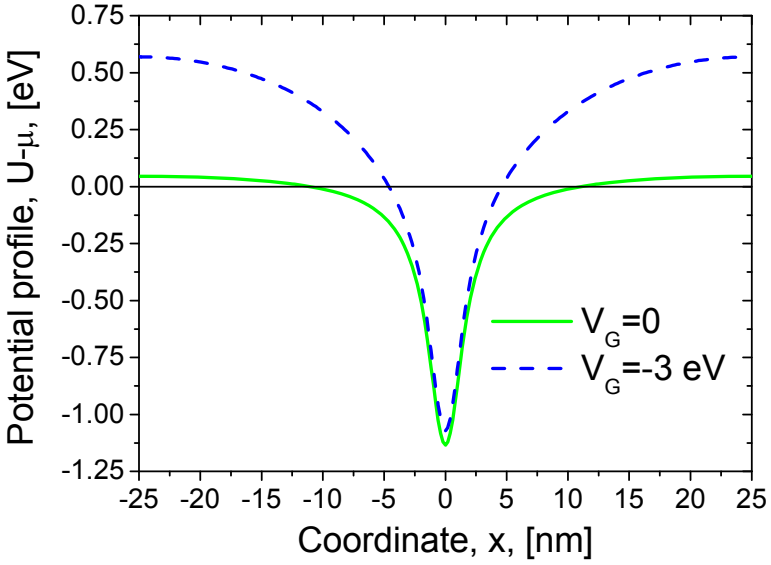

Figure 2. The spatial distributions of potential energy in the source-drain direction for different gate voltages V_G at T=300K. The Fermi level is indicated by a horizontal solid line.

The potential barrier height referenced to the Fermi level vs. gate voltage for different temperatures is presented in Fig. 3. For negative gate voltage the Fermi level is steadily deepened into the potential well. It should be emphasized that the dependence of the barrier height on the temperature is rather strong that leads to substantial increase in the sensitivity of the feasible bolometer based on the structure under consideration.

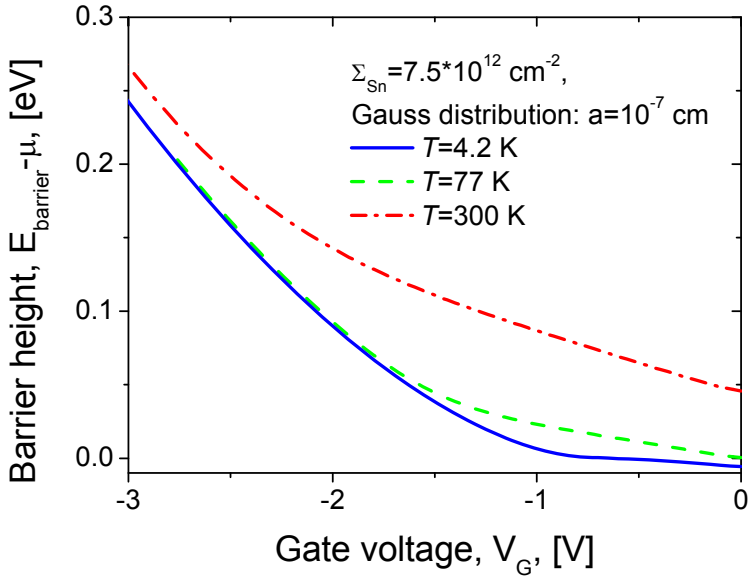

Figure 3. Potential barrier in nanothreads with respect to the Fermi level (the localization energy) vs. gate voltage for different temperatures.

The fraction of delocalized electrons with respect to their total number vs. gate voltage for different electron temperatures is presented in Fig. 4. The Figure confirms an expectation that negative gate voltage enhances anisotropy of conductivity which is crucial for the possible application as a bolometer. For zero gate voltage (that is in absence of gate and open surface) the anisotropy is rather small that is also in accordance with previous experimental data [1, 2].

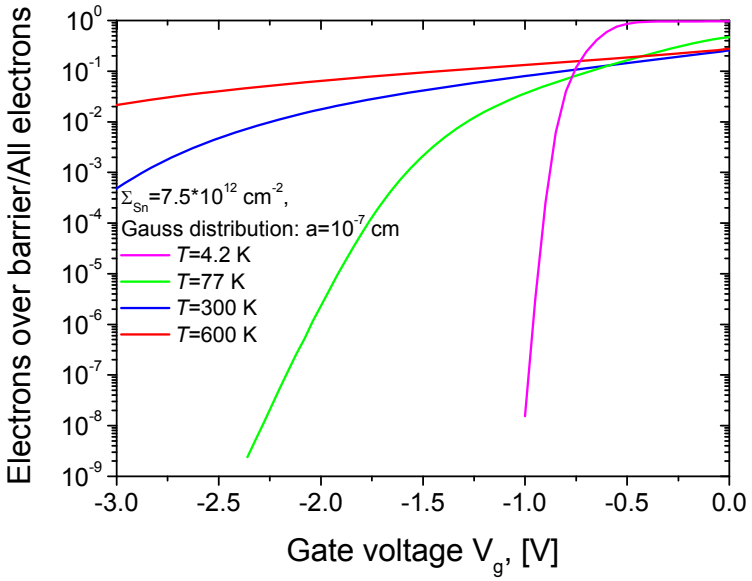

Figure 4. Fraction of delocalized electrons vs. gate voltage for different temperature T.

We have examined the fraction of delocalized electrons vs. gate voltage at room temperature for different Gaussian parameter *a* (Fig. 5). Below it will be used to choose the value of parameter *a* providing the best concordance with experimental I-V curves. The dependency for delta-function practically coincides with that for the parameter $a=10^{-7}$cm, that confirms a validity of the model with delta-function in the case.

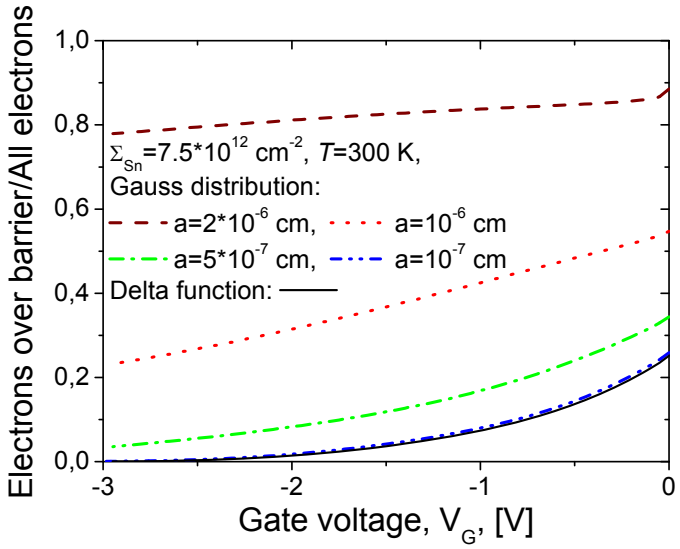

Figure 5. Fraction of delocalized electrons vs. gate voltage at room temperature for different Gaussian parameter *a* and delta-function.

The mean electron sheet density vs. gate voltage for different temperatures is quite linear and weakly depends on temperature (Fig. 6). This manifests a validity of a simple model of a plate capacitance to evaluate a mean electron density. It is due to a quite large distance from the gate to nanothreads, namely, 50 nm.

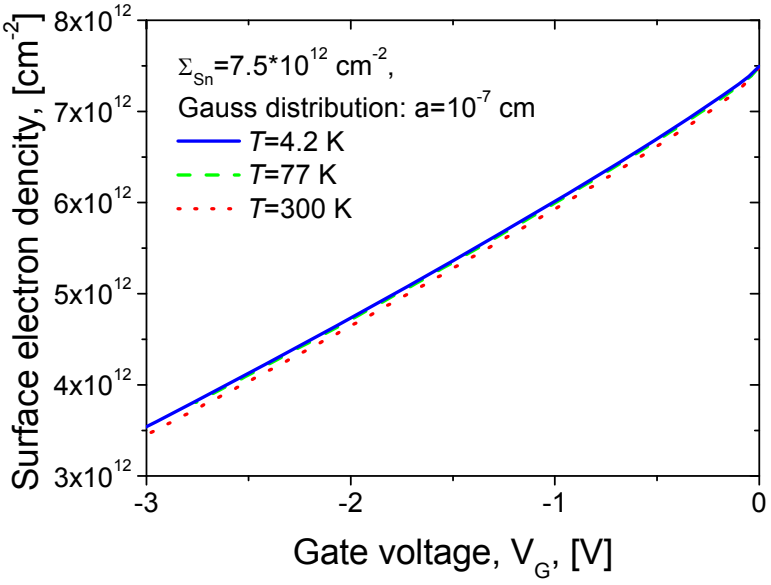

Figure 6. The mean electron density vs. gate voltage for different temperatures.

4. QUANTUM SIMULATION

The quantum model is based on self-consistent solution of 2D Schrödinger equation and 2D Poisson equation. The model accounts for the quantization of the electron energy spectrum in the self-consistent two-dimensional electric potential, herewith the electron density distribution in nanothread arrays for different gate voltages was calculated. The electrons are distributed over energy levels according to Fermi-Dirac statistics. It turned out that qualitatively both models demonstrate similar behavior, nevertheless, the classical one is in better quantitative agreement with experimental data.

The simulated potential energy profile and energy levels are depicted in Fig. 7 for zero gate voltage and in Fig. 8 for the gate voltage equal to -1.4 V. There the Fermi level is attached to zero energy. Fig. 9 represents the portion of delocalized electrons against the gate voltage. The non-monotonic behavior of this function with respect to the gate voltage must become apparent in measured I-V curves. This non-monotonic behavior could be interpreted as a result of states are thrown out over the Fermi level at the gate voltage V_g=-1.4 V (Fig. 8) compared to that at V_g= 0 V (Fig. 7). However, nothing of the kind is visible in experimental curves (Fig. 10) Plausibly, the quantization could be ignored because Sn atoms are randomly distributed along the thread axis in fabricated structures.

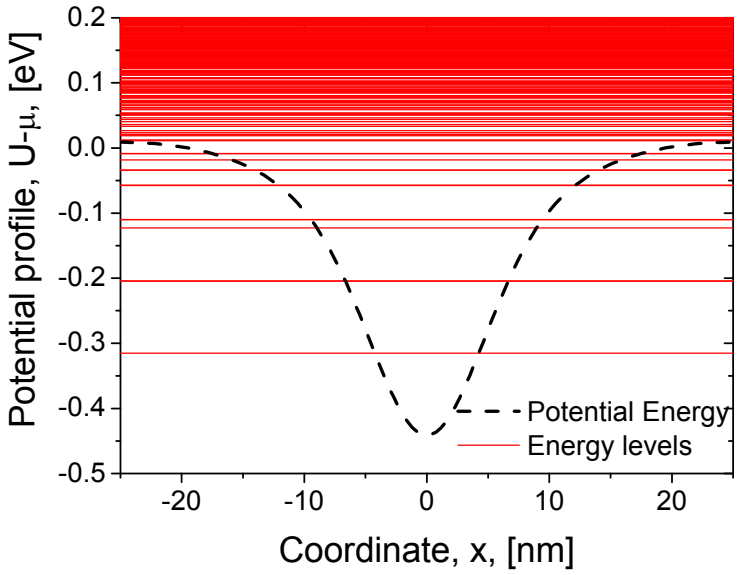

Figure 7. Potential energy profile (dashed line) and energy levels (solid lines) for zero gate voltage. The Fermi level is referenced to zero energy.

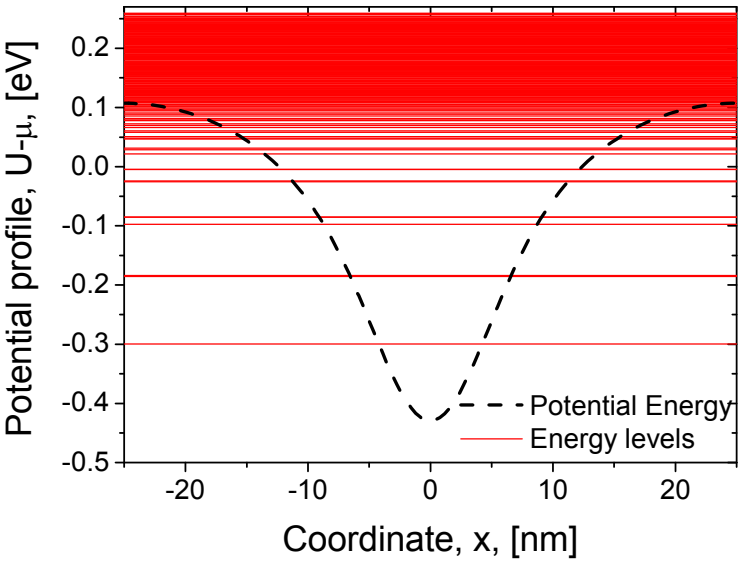

Figure 8. Potential energy profile (dashed line) and energy levels (solid lines) for the gate voltage equal to -1.4 V. The Fermi level is positioned at zero energy.

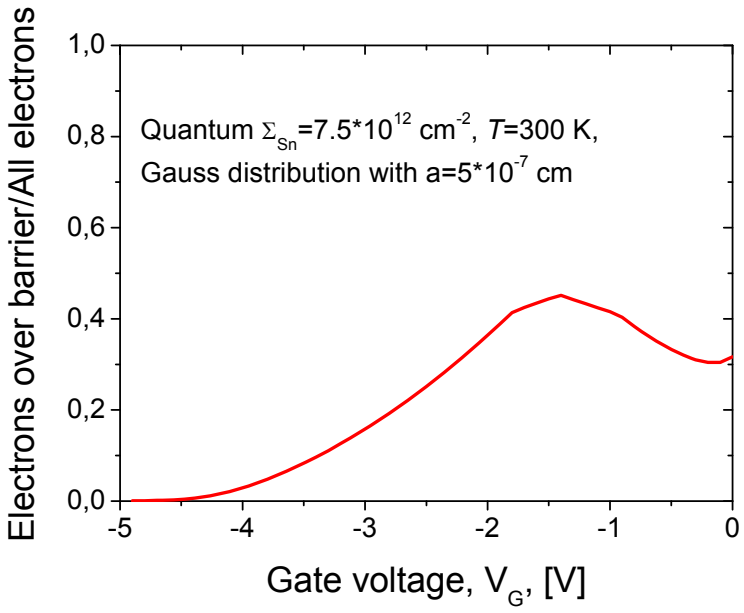

Figure 9. Fraction of delocalized electrons vs. gate voltage at room temperature according to quantum model.

5. COMPARISON WITH EXPERIMENT

The series of I-V curves at room temperature T=300 K was measured in the experiment. The extracted curves correspond to fairly low drain voltage 0.5 V and different direction of current, they are presented in Fig. 10. The anisotropy of current, parallel to nanothreads (PAR) and perpendicular (PERP) to them, is remarkably augmented for negative gate voltage. This is in a qualitative agreement with results of simulation in Fig. 4.

However, to achieve a quantitative concordance one has to suggest that a mobility μ_d of delocalized electrons and the mobility μ_t of electrons localized in nanothreads are different. In the case the coefficient of anisotropy equal to the ratio $(I_{par}- I_{perp})/I_{perp}$ is

$$\frac{I_{par}-I_{perp}}{I_{perp}}=\frac{\mu_t}{\mu_d}\frac{1-F}{F}, \tag{8}$$

where I_{par} is a current parallel to nanothreads, I_{perp} is a current perpendicular to nanothreads, $F(Vg, T)$ is the fraction of the delocalized electrons with respect to all electrons. There are two parameters to fit the theory (Fig. 4) into experimental data (Fig. 10), i.e. the Gaussian dispersion factor a and the ratio of mobilities μ_t/μ_d. The best concordance is provided by a= 1 nm, whereas the lattice constant is around 0.5 nm. Worth noting that bigger values of the parameter a cannot explain at all the high anisotropy of conductance experimentally observed in the structure. This could be regarded as an indirect confirmation of existence of Sn-nanothreads.

The ratio of mobilities μ_t/μ_d=1/40 for V_g=0 V and μ_t/μ_d=1/10 for V_g=-3 V which is looking quite reasonable as the average bulk concentration of Sn impurities in nanowires (taking into account the electron confinement length of 10 nm at the Fermi level) amounts to extremely large value 5 10^{19}cm^{-3}. The difference in ratios could be explained by the fact that the impurity potential is stronger screened by electrons in nanothreads at V_g=0 V.

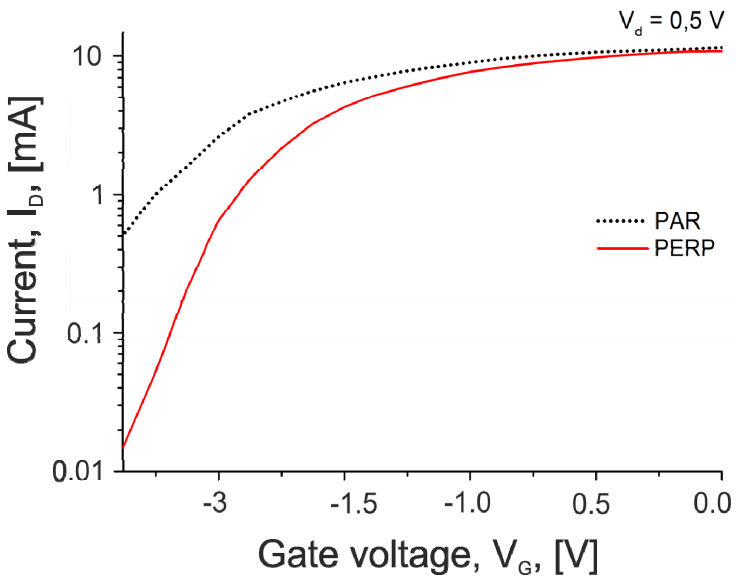

Fig. 10. Extraction from series of measured I-V curves: current vs. gate voltage at low drain voltage (V_d=0.5 V) for current flow perpendicular to nanothreads (PERP) and parallel to them (PAR).

The operation of a THz hot-electron bolometer based on the proposed structure could be associated with heating of electrons in nanothreads resulting in an increase in delocalized electrons and, hence, an increase of current perpendicular to nanothreads [3]. Many types of bolometers based on different nanostructures were put forward previously: on quantum dots [4], on quantum wells and quantum wires [5], on nanotubes [6], on thin superconducting films [7].

6. CONCLUSIONS

The gated GaAs structures resembling the field-effect transistor with the array of the Sn nanothreads.was fabricated and series of I-V curves was measured. Two device models for simulation were developed. The quantum model accounts for the quantization of the electron energy spectrum in the self-consistent two-dimensional electric potential, providing the electrons are distributed over the energy levels in accordance with the Fermi-Dirac statistics. The classical model ignores the quantization and electrons are distributed in space according to 3D density of states and Fermi-Dirac statistics. It turned out that qualitatively both models demonstrate quite similar behavior, nevertheless, the classical one is in much better quantitative agreement with experimental data. Plausibly, the quantization could be ignored because Sn atoms are randomly distributed along the thread axis.

Only comparison of simulated plots with experimental I-V curves allows revealing the invisible physical parameters of the structure. Namely, the Sn atoms are randomly distributed along nanothread axis with dispersion about 1 nm, the electrons are localized in nanothreads at distances about 10 nm. In fact, this is the only indirect confirmation of nanothreads existence. The mobilities of localized and delocalized electrons markedly differ (by tens). The latter is explained by rather heavy random doping in nanothreads.

The terahertz hot-electron bolometers (HEBs) could be based on the structure under consideration. Its operation is associated with heating of electrons in nanothreads by incident THz radiation resulting in an increase in delocalized electrons and, hence, an increase of current perpendicular to nanothreads. A high polarization selectivity of the bolometer seems plausible: whether electric field is parallel or perpendicular to the threads.

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REFERENCES

[1] Khabibullin R. A., Yachmenev A. E., Lavrukhin D. V., Ponomarev D. S., Bugayev A. S. and Maltsev P. P., "Pseudomorphic HEMT with Sn nanowires on a vicinal GaAs substrate". Semicond. Sci. Technol. 30, 085009 (2015).
[2] Khabibullin R.A., Yachmenev A.E., Lavrukhin D.V., Ponomarev D.S., Bugayev A.S., and Maltsev P.P., "Electron Transport and Optical Properties of Structures with Atomic Tin Nanowires on Vicinal GaAs Substrates," Semiconductors 50, 185–190 (2016).
[2] Semenikhin I., Vyurkov V., Bugaev A., Khabibullin R., Ponomarev D., Yachmenev A., Maltsev P., Ryzhii M., Otsuji T., and Ryzhii V., "Terahertz bolometer based on Sn nanothreads in GaAs," Proc. Int. Conf. Micro- and Nanoelectronics (ICMNE'2016) Book of Abstracts, Moscow – Zvenigorod, Russia, 142 (2016).
[3] Ryzhii V., "The theory of the quantum-dot infrared phototransistors," Semicond. Sci Technol. 11, 759 (1996).
[4] Ryzhii V., Khmyrova I., Ryzhii M., and Ershov M., "Comparison studies of infrared phototransistors with a quantum-well and a quantum-wire base," J. Physique IV, Colloque 3, suppl. J. Physique III 6, C3157 (1996).
[5] Gayduchenko I.A., Fedorov G.E., Stepanova T.S., Titova N., B.M. Voronov, But D., Coquillat D., Diakonova N., Knap W., and Goltsman G.N.. "Asymmetric devices based on carbon nanotubes as detectors of sub-THz radiation," Journal of Physics: Conference Series 741, 012143 (2016).
[6] Seliverstov S.V., Rusova A.A., Kaurova N.S., Voronov B.M., and Goltsman G.N. "Attojoule energy resolution of direct detector based on hot electron bolometer." Journal of Physics: Conference Series 741, 012165 (2016).