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Effect of "Mexican Hat" on Graphene Bilayer Field-Effect Transistor Characteristics

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Ballistic model of a graphene bilayer field-effect transistor (GBL FET) was developed. It incorporates the exact graphene bilayer electronic spectrum reminding a "Mexican hat". The isotropic minimum shifted from the center of a band results in a conductance step at low temperature which was so far known for one-dimensional conductors due to conductance quantization. At room temperature a GBL FET exhibits an extremely high transconductance in ON-state. It makes a GBL FET promising for high-frequency analog circuits. We also point out to possibility of electron localization inside the channel on the top of potential barrier. () 2011 The Japan Society of Applied Physics

1. Introduction

Carbon-based materials are intensively investigated with prospects of their future application in electronics and optoelecronics. Compared to graphene monolayer the graphene bilayer (GBL) possesses a field-tunable bandgap. Most of theoretical papers are just devoted to bandgap engineering.^{1,4,6)} Indeed, the gap could be much augmented with increasing transversal electric field ($\Delta = 0.2 \text{ eV}$ at 10^{10} V/m^{1}).

Semianalytical models of a ballistic double-gate GBL field-effect transistor (FET) were recently developed. In ref. 2 the characteristics of GBL FET were derived using the Boltzmann equation in two limits: ballistic transport and strongly collisional transport. The transconductance of GBL FET in ac and dc regimes was analyzed. However, an electronic spectrum was simplified and considered as parabolic one with a constant effective mass independent of transversal electric field.

A semianalytical model of a ballistic GBL FET with an exact spectrum was presented in ref. 3. However, the authors paid no attention to the impact of GBL spectrum features on FET characteristics. The latter is the main goal of the present communication. In particular, we emphasize the unusual filling of different branches of spectrum inside the channel and existence of localized states which do not contribute to current. All that makes the ballistic model of a GBL FET non-trivial compared to conventional semiconductors and graphene monolayer.

2. The Exact GBL Spectrum and Its Approximations

The dispersion law of bilayer graphene calculated in tightbinding approximation is¹⁾

$$\varepsilon = \pm \sqrt{\frac{\gamma_1^2}{2} + \frac{\Delta^2}{4} + v^2 p^2} \pm \sqrt{\frac{\gamma_1^4}{4} + v^2 p^2 (\gamma_1^2 + \Delta^2)} \quad (2.1)$$

with numerical values of parameters herein: $\gamma_1 = 0.39 \text{ eV}$, $v = 8 \times 10^5 \text{ m/s}$, the parameter Δ (the levels assymetry) being dependent on the transversal electric field. The outer sign corresponds to electrons and holes, the inner sign belongs to two branches of spectrum: the lower one, to some extent, reminds a "Mexican hat" and the higher one

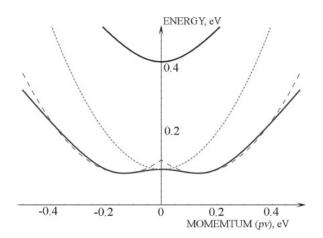


Fig. 1. Electronic spectrum of bilayer graphene (solid), parabolic approximation in the vicinity of p_{\min} (dashed) and parabolic spectrum with effective mass $m = 0.053m_e$ (dotted).

is a quite parabolic valley. The exact dispersion law for electrons is depicted with solid lines in Fig. 1 for the parameter $\Delta = 0.2 \text{ eV}$. In the same figure there are also depicted the parabolic approximation to the spectrum in the vicinity of the band minimum (dashed line) and the parabolic approximation with effective mass $m = 0.053m_{\text{e}}$ employed in ref. 2 (dotted line). The exact curve has a minimum at

$$p_{\min} = \frac{\Delta}{2v} \sqrt{\frac{2\gamma_1^2 + \Delta^2}{\gamma_1^2 + \Delta^2}},$$
(2.2)

while the corresponding energy is

$$\varepsilon(p_{\min}) \equiv \varepsilon_{\min} = \frac{\gamma_1 \Delta}{2\sqrt{\gamma_1^2 + \Delta^2}},$$
 (2.3)

therefore, the gap is

$$\Delta_g \equiv 2\varepsilon_{\min} = \frac{\gamma_1 \Delta}{\sqrt{\gamma_1^2 + \Delta^2}}.$$
 (2.4)

Further we accept the parameter Δ to be equal to 0.2 eV. To sustain this value the direct voltages of approximately ± 10 V must be applied to the top and back gates. At the same time, the operational gate voltages may be much lower.

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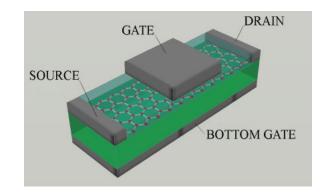


Fig. 2. (Color online) Schematic view of a transistor under simulation.

3. Analytical Ballistic Model of GBL FET: Low Drain Voltage, Low Temperature

An analytical model of a graphene bilayer field-effect transistor was developed. For a while, we restrict our discussion by infinitesimal drain voltages and low temperature to derive the analytical expressions for conductivity. The transistor under consideration is sketched in Fig. 2. For numerical evaluations we shall use the following parameters of the transistor: the top gate oxide thickness is $d_1 = 1$ nm, the back gate oxide thickness is $d_2 = 10$ nm, the permittivity of top and bottom gate insulators is $\kappa_1 = \kappa_2 = 4$. The relevant electrostatic equations are

$$\begin{cases} E_1 d_1 + E_2 d_2 = V_{\rm G}, \\ \kappa_1 E_1 - \kappa_2 E_2 = 4\pi e n(V_{\rm C}, T), \\ E_2 d_2 = V_{\rm C}, \end{cases}$$
(3.1)

where E_1 and E_2 are electric fields under the top gate and above the back gate, respectively, V_G is a top gate potential, the back gate potential is supposed to be equal to zero, *n* is a sheet density of electrons in the channel, V_C is a channel potential. In fact, it determines the height of potential barrier between source/drain and channel when they are sustained at zero voltage. Evidently, the potential barrier height with respect to the drain and source contacts is varied by applied voltages. Taking into account that commonly a top gate dielectric is much thinner than that of the back gate $(d_1/d_2 \ll 1)$ one arrives at the solution

$$V_{\rm G} = V_{\rm C} + \frac{4\pi e d}{\kappa_1} n(V_{\rm C}, T).$$
 (3.2)

Hereafter, the goal is to invert this equation, i.e., to obtain the dependence $V_{\rm C}(V_{\rm G})$. The calculation of density $n(V_{\rm C})$ can be performed analytically for zero temperature T = 0, more strictly, for fairly low temperature when the inequality: $kT \ll eV_{\rm DS}$ is valid, where $V_{\rm DS}$ is a source–drain voltage. Before the immediate calculations one should pay attention to an unusual phenomenon which can occur due to peculiarities of GBL spectrum. For the sake of clarity we discuss the situation when the Fermi level in source and drain contacts is placed fairly above the cap. The states of electrons belonging to the cap of Mexican hat can be localized inside the channel although there is a potential barrier instead of a potential well. In the case those states contribute to the charge density but do not contribute to the current. Electrons with sufficiently low energy belonging to

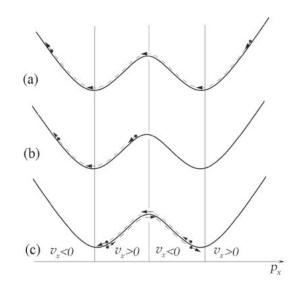


Fig. 3. Motion of electrons along the dispersion curve: brim electrons are backscattered from the potential barrier (a), cap electrons are backscattered (b), and cap electrons are localized in the channel (c).

brims are backscattered from the potential barrier and return to the contact. In Fig. 3(a) their motion along the dispersion curve is indicated. The sign of group velocity defines the direction of motion in space, zero velocity in extrema of the dispersion curve corresponds to stationary points. Analogously, electrons belonging to the cap are also backscattered and return to the contact [Fig. 3(b)]. After a positive voltage is applied to gates the electrons belonging to brim states in the contact with fairly high energy surmount the barrier and penetrate into the channel. The associated brim states inside the channel become occupied after the transition time elapsed. The cap states inside the channel can be occupied after much larger time passed due to scattering of brim electrons. The cap states are localized inside the channel. Their motion to and fro along the dispersion curve is indicated in Fig. 3(c). As we are accentuated on high frequency behavior of GBL FET, further we suppose the cap states to be empty inside the channel. In this case the density is

$$n(V_{\rm C}) = e \int_{p_{\rm min}}^{\infty} \frac{2\pi gp \, dp}{(2\pi)^2} f_{\rm F}(\varepsilon(p)), \tag{3.3}$$

where g = 4 is the electronic degeneracy factor in graphene, including spin and band degeneracy, and f_F is the Fermi distribution function. At T = 0 one easily obtains

$$u(V_{\rm C}) = \frac{e^2}{\pi \hbar^2 v^2} \bigg[(\mu - eV_{\rm C})^2 - \varepsilon_{\rm min}^2 + \sqrt{\gamma_1^2 + \Delta^2} \sqrt{(\mu - eV_{\rm C})^2 - \varepsilon_{\rm min}^2} \bigg].$$
(3.4)

It follows the above equation that when the chemical potential μ "touches" the bottom of the conductance band the carriers fill the channel [see Fig. 4(b)]. If $(\mu - eV_C) < \varepsilon_{\min}$ there are no carriers in the channel [and thus no screening, see Fig. 4(a)]. Then eq. (3.2) gives rise to the evident equality $V_C = V_G$. For the sake of simplicity, we suppose that the position of Fermi level in the channel corresponds to the middle of a gap when zero voltage is applied to the top gate ($V_G = 0$). The conductance is

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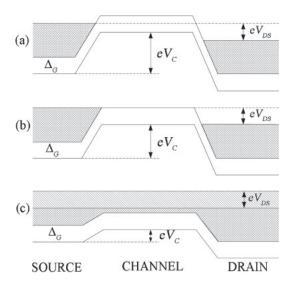


Fig. 4. Band diagrams for the transistor: (a) OFF-state, (b) threshold, (c) ON-state.

caused by the contribution of electrons in a narrow energy interval between Fermi levels of source $\mu_{\rm L}$ and drain $\mu_{\rm R}$, $\mu_{\rm L} - \mu_{\rm R} = eV_{\rm DS}$. Among them only electrons with positive group velocities should be selected. After that the formula for the current caused by infinitesimal source–drain voltage $dV_{\rm DS}$ is

$$dj = e \langle v_x \, dn \rangle = e \int_{\substack{v_x > 0\\\varepsilon \in [\mu_L; \, \mu_R]}} g v_x \frac{d^2 p}{(2\pi\hbar)^2}. \quad (3.5)$$

Introducing the x-component of the group velocity as

$$v_x = \frac{d\varepsilon}{dp_x} = \frac{d\varepsilon}{dp}\cos\theta,\tag{3.6}$$

one easily arrives at the expression for the current

$$dj = \frac{ge}{(2\pi\hbar)^2} \int_{-\pi/2}^{\pi/2} d\theta \int_{p(\mu_{\rm L})}^{p(\mu_{\rm R})} \frac{d\varepsilon}{dp} \cos\theta p \, dp \, d\theta$$
$$= \frac{2ge^2 p(eV_{\rm C}) \, dV_{\rm DS}}{(2\pi\hbar)^2}.$$
(3.7)

The conductance as a function of channel potential is

$$G = \frac{e^2}{h} \frac{gk(eV_{\rm C})}{\pi}.$$
(3.8)

In general, the function $k(eV_C) = p(eV_C)/\hbar$ could be manifold, but, as it was mentioned above, the states on the cap are supposed to be empty. Equation (3.8) leads to a conclusion that a conductance of a BLG FET exhibits a step at $eV_C = \varepsilon_{\min}$. An explicit analytical formula for the value of step reads

$$\Delta G = \frac{e^2}{h} \frac{gk_{\min}}{\pi}.$$
(3.9)

For $\Delta = 0.2 \,\text{eV}$ the wave vector $k_{\min} = 4 \,\text{nm}^{-1}$ and the conductance step is $\Delta G = 1.25 \times 10^4 \,(\Omega \cdot \text{m})^{-1}$. Worth mentioning the conductance step is not restricted by the conductance quantum as it is proportional to the channel width.

GBL is a unique semiconductor with an isotropic minimum shifted from the center of a band $(k_{\min} \neq 0)$. Just

this kind of minimum results in a conductance step at low temperature. To our best knowledge, we firstly report about a possibility of a conductance step in two-dimensional (2D) systems. So far it was known only in one-dimensional (1D) conductors (due to conductance quantization).

In general, the conductance is proportional to the product of density of states and group velocity. Therefore, for 1D conductors it is constant no matter what is a spectrum. For 2D conductors with isotropic spectrum the shifted minimum is crucial for existence of a conductance step. All conventional semiconductors (silicon, germanium, A3B5) possess anisotropic shifted minima. An isotropic parabolic minimum in the center of band in 2D systems of common semiconductors results in a constant density of states. For graphene monolayer with linear spectrum the density of states is equal to zero at the band edge. For both cases no conductance step seems possible. One more feature of GBL is that the density of states at the band edge in GBL reveals a singularity $\varepsilon^{-1/2}$. It originates in both circumstances: a shifted isotropic minimum and a parabolic spectrum in the vicinity of it. Amazingly, this singularity is the same as in a semiconductor carbon nanotubes, therefore, the behavior of the GBL channel reminds, to some extent, that of an array of nanotubes. The singularity may be also important for optoelectronic applications of GBL structures.

Potentially, eq. (3.8) could be used for calculation of conductance G with respect to an arbitrary gate voltage V_G at zero temperature. However, this problem requires the solution of a 4th order algebraic equation.

4. Semianalytical Ballistic Model of GBL FET: Arbitrary Drain Voltage, Arbitrary Temperature

In case of arbitrary temperature the Fermi–Dirac distribution function is engaged in the expressions for the charge density and current. Herewith, for fairly small gap and/or fairly high temperatures the hole contribution to the current and charge may become substantial. Therefore, the charge density is

$$n(V_{\rm C},T) = \frac{2}{\pi\hbar^2 v_{\rm F}^2} \int_{q_{\rm min}}^{\infty} [f_{\rm F}(\varepsilon,V_{\rm C}) - f_{\rm F}(\varepsilon,-V_{\rm C})] q \, dq, \quad (4.1)$$

where $q = pv_F$ and the second term corresponds to holes. If a finite drain-source voltage V_{DS} is applied the system of electrostatic equation (3.2) should be properly modified:

$$\begin{cases} E_1 d_1 + E_2 d_2 = V_{\rm G}, \\ \kappa_1 E_1 - \kappa_2 E_2 = 4\pi e \cdot \frac{1}{2} [n(V_{\rm C}) + n(V_{\rm C} - V_{\rm DS})], \\ E_2 d_2 = V_{\rm C}, \end{cases}$$
(4.2)

where $n(V_{\rm C})$ is a density caused by electrons moving from the source (left) contact, while $n(V_{\rm C} - V_{\rm DS})$ is a density caused by electrons moving from the drain (right) contact. The upgraded expression for current is

$$j = \frac{2eg}{(2\pi\hbar)^2} \int_{-\infty}^{\infty} [f_{\rm F}(\varepsilon, V_{\rm C}) - f_{\rm F}(\varepsilon, V_{\rm C} - V_{\rm DS})] p(\varepsilon) \, d\varepsilon. \quad (4.3)$$

The lower limit of integration equal to $-\infty$ means that holes are involved into consideration due to identity of electron and hole spectra in graphene and its modifications. This equation can be integrated numerically. For the infinitesimal drain-source voltage one can make a substitution

$$f_{\rm F}(\varepsilon, V_{\rm C}) - f_{\rm F}(\varepsilon, V_{\rm C} - V_{\rm DS}) = -\frac{df_{\rm F}}{d\varepsilon} V_{\rm DS} \qquad (4.4)$$

and obtain the conductance

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$$G = \frac{dJ}{dV_{\rm DS}} = \frac{2e^2gp_{\rm min}}{(2\pi\hbar)^2} \left[f_{\rm F}(\varepsilon_{\rm min}, V_{\rm C}) + f_{\rm F}(-\varepsilon_{\rm min}, V_{\rm C}) \right] + \frac{2e^2g}{(2\pi\hbar)^2} \int_{p_{\rm min}}^{\infty} \left[f_{\rm F}(\varepsilon, V_{\rm C}) + f_{\rm F}(-\varepsilon, V_{\rm C}) \right] dp$$

$$(4.5)$$

This equation consists of two parts. One of them attributes to an isotropic shift of GBL spectrum. Just this part results in existence of a conductance step (3.8). Evidently, it eliminates when $p_{\min} = 0$. The second part survives for unshifted parabolic spectrum $\varepsilon(p) \sim p^2$. The dependencies of conductance vs gate voltage $G(V_G)$ were calculated numerically using eqs. (4.5) and (4.1) for different temperatures: T = 4, 77, and 300 K (Fig. 5). The current vs gate voltage curves $j(V_G)$ for the source–drain voltage $V_{DS} =$ 0.2 V are presented in Fig. 6. The most striking feature of those curves is a high transconductance near the threshold voltage which is an item of the next section.

5. Transconductance

In fact, the transconductance g_m of GBL FET at T = 0 near threshold is infinite for both shifted and unshifted parabolic spectrum models although the strength of singularity is different. The goal of this section is to prove that the shift of the band minimum leads to an unusual dependence of conductance $g_m(T)$ upon temperature: the common law $g_m \sim T^{-1}$ is no more valid. To estimate the transconductance analytically one can use the following equations:

$$e\Delta V_{\rm C} = kT,\tag{5.1}$$

$$g_{\rm m} = \frac{\partial I_{\rm D}}{\partial V_{\rm G}} \approx \Delta G W \cdot \frac{e V_{\rm DS}}{\Delta V_{\rm G}}, \qquad (5.2)$$

where $\Delta V_{\rm C}$ denotes the shift of the Fermi level from the bottom of the conductance band, W is the channel width, and k is the Boltzmann constant. Equation (5.1) defines the energy interval of the occupied electron states at $T \neq 0$ when the level of chemical potential touches the bottom of the conduction band (i.e., at the threshold voltage). This is just the case when the transconductance as a function of gate voltage $V_{\rm G}$ attains its maximum. The next step is to derive the dependence of $V_{\rm C}$ over $V_{\rm G}$. In comparison with general equation (4.1) the task is much simplified owing to eq. (5.1). In eq. (4.1) one should

- substitute $\varepsilon_{\min} + \Delta V_{\rm C} = \varepsilon_{\min} + kT$ instead of $V_{\rm C}$;
- expand $\varepsilon(q)$ in series of powers of $(q q_{\min})$;
- neglect the hole contribution.

After that the expression for the carrier concentration is

$$n(V_{\rm C},T) = \frac{2}{\pi\hbar^2 v^2} \int_{q_{\rm min}}^{\infty} \left\{ 1 + \exp\left[\frac{(q-q_{\rm min})^2}{2mv^2kT} - 1\right] \right\}^{-1} q \, dq,$$
(5.3)

where *m* is the effective electron mass in the vicinity of $p = p_{\min}$, defined by the following equation:

$$m = \frac{\gamma_1 (\gamma_1^2 + \Delta^2)^{3/2}}{2v^2 \Delta (2\gamma_1^2 + \Delta^2)}.$$
 (5.4)

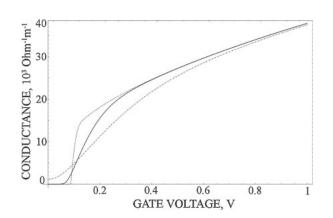


Fig. 5. Conductance vs gate voltage: T = 300 (solid), 77 (dotted), and 4 K (dot-dashed).

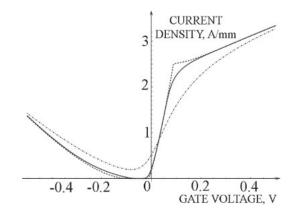


Fig. 6. Current density vs gate voltage for $V_{\rm DS} = 0.2$ V: T = 300 (solid), 77 (dotted), and 4 K (dot-dashed).

Equation (5.3) can be taken analytically. After substituting its value to the eq. (3.2) one obtains

$$eV_{\rm G} = \varepsilon_{\rm min} + kT + \frac{8e^2d}{\kappa_1\hbar^2} \times \left[\ln(1+e)mkT + 0.91q_{\rm min}\sqrt{\frac{2mkT}{v^2}}\right], \quad (5.5)$$

where 0.91 is an approximate value of the integral

$$\int_0^\infty \frac{dt}{1 + e^{t^2 - 1}}.$$
 (5.6)

Shortly, the value of smearing can be presented as

$$\Delta V_{\rm G} = aT + b\sqrt{T},$$

where a and b are functions of both spectrum and structure parameters. For the above mentioned structure parameters we obtain (here T is expressed in eV)

$$\Delta(eV_{\rm G}) = 4.266T + 0.8775\sqrt{T},\tag{5.7}$$

$$\frac{dG}{dV_{\rm G}} = \frac{\Delta G(T=0)}{4.266T + 0.8775\sqrt{T}}.$$
 (5.8)

Two important conclusions originate from eqs. (5.5) and (5.8):

- The influence of charge in the channel is important;
- The shift of spectrum minimum results in the term proportional to \sqrt{T} in eq. (5.8) which does not exist for simplified parabolic spectrum.

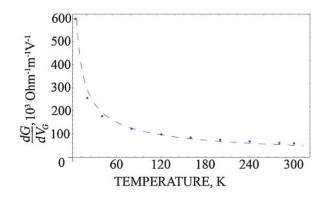


Fig. 7. (Color online) Transconductance as a function of temperature for the threshold gate voltage.

At room temperature both terms in eq. (5.8) turned out to be of the same order of magnitude, while at low temperatures the second one dominates. The next question examined was the agreement between the analytical formula (5.8) and numerical calculations based on the exact spectrum. In advance, one could not expect a good agreement between those two approaches because the assumption (5.1) is not really rigorous. However, the result depicted in Fig. 7 demonstrates a good agreement between numerical (dots) and analytical (dashed curve) calculations in spite of apprehensions. A simple analysis reveals that the maximum transconductance is an increasing function of the parameter of level asymmetry Δ which is dependent on a transversal electric field. However, Δ cannot surpass the interlayer interaction constant γ_1 . A comparison of conductance calculated for exact GBL spectrum and its parabolic approximation used in ref. 2 is presented in Fig. 8. Near the threshold gate voltage there is a substantial difference at low temperature and quite good coincidence at high temperature. The mismatch for high gate voltage at any temperature is attributed to almost linear behavior of exact spectrum for high energy. For $\Delta = 0.2 \,\text{eV}$ the transconductance dG/dV_G at room temperature obtained via numerical calculations is $63 \times 10^3 \Omega^{-1} m^{-1} V^{-1}$. The analytical calculation based upon eq. (5.8) gives $55 \times 10^3 \Omega^{-1} \mathrm{m}^{-1} \mathrm{V}^{-1}$. This value is by an order greater than that for an ultrathin body fully depleted silicon-on-insulator FET (5×10^3) $\Omega^{-1} \operatorname{m}^{-1} V^{-1}$) which is regarded as the most prospective in silicon electronics.⁵⁾

6. Conclusions

Analytical and semianalytical ballistic models of a fieldeffect transistor for the exact graphene bilayer spectrum were developed. Even at high transversal electric fields when a band gap achieves 0.2 eV this type of transistor does not reveal a sufficiently big ON/OFF ratio. However, its high transconductance ($\approx 5 \times 10^4 \,\Omega^{-1} \,\mathrm{m^{-1}} \,\mathrm{V^{-1}}$ at room temperature) opens prospects to applications in analog circuits. Unlike to other ballistic field-effect transistors, the transconductance could be much augmented at lower temperature. The conductance exhibits an abrupt jump at low

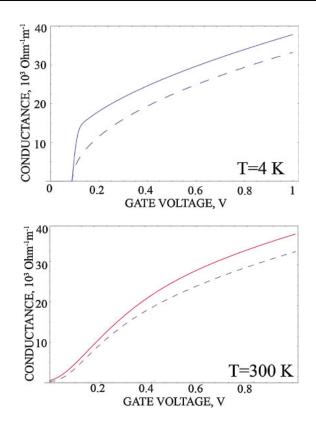


Fig. 8. (Color online) Conductance vs gate voltage: exact spectrum (solid) and unshifted parabolic approximation (dashed).

temperature near the threshold gate voltage. To our best knowledge, graphene bilayer is a unique two-dimensional material where a conductance step is possible. So far, such a phenomenon was known only for one-dimensional conductors due to conductance quantization. The step originates in an isotropic minimum in spectrum shifted from the center of band (Mexican hat). An attention was also paid to a possibility of localization of electrons on a potential barrier top inside a channel. Plasma oscillations in such a resonator excited by a current seem plausible.

Acknowledgments

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SELECTED TOPICS IN APPLIED PHYSICS



Dmitry Svintsov received B.S. degree in applied mathematics and physics from Moscow Institute of Physics and Technology (Technical University), Moscow, Russia, now is finishing the MS course at the same university. His current interest lies in theory and simulation of carbon-based electronic devices.



Vladimir Vyurkov received M.S. degree in electronic devices from Moscow Institute of Physics and Technology (Technical University), Moscow, Russia, in 1975 and the Ph. D. degree in physics and mathematics from the same Institute in 1978. From 1978 to 1985 he worked for Kurchatov Atomic Energy Institute, Moscow, from 1985 to 1989 he was a senior researcher at the Institute of Electric Sources, Moscow, from 1989 to present he is a leading researcher at the Institute of Physics and

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Victor Ryzhii has been a Professor of the University of Aizu, Japan, since 1993. He obtained his Ph. D. and Doctor of Science degrees from Moscow Institute of Physics and Technology, Russia, in 1970 and 1975, respectively. His research activity is associated with physics and computer modelling of low-dimensional semiconductor heterostructures and electron, optotoelectron, and terahertz devices based on nanostructures, including graphene-based devices. He has about 300 journal

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