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***Abstract*—Modeling results of planar 2D/3D semiconductor heterostructure based on GaN/MoS_2 junction are presented. The heterostructure represents a III-nitride based planar diode with length of 1 μm. The diode has a GaN n-type channel and MoS_2 layer placed at the bottom and connected to anode contact. Doping concentration in the channel is $(1–6)\cdot10^{22}m^{-3}$. Model of electron exchange between 2D and 3D regions of the diode is proposed. Electron transition between 2D and 3D region of diode is suggested to occur due to polar optical phonon scattering. Monte Carlo simulation of electron transport in device is carried out. Dependences of current density on applied voltage are obtained. Impact of parameters of MoS_2 layers on current – voltage characteristic of diodes is discussed.**

Keywords—two-dimensional(2D) layer, heterojunction, electron transfer, phonon scattering, current density, I-V-characteristic.

I. INTRODUCTION

Two-dimensional (2D) semiconductors are considered as perspective materials for novel electronic devices. Well known monolayer materials as graphene was first of them. Today, other 2D materials are extensively investigated. For example, hexagonal transition metal dichalcogenides (TMDCs) [1,2], black phosphorus (BP) [3,4] et. al. Usage of vertical 2D – based heterostructures allows to create 2D analoges of most original devices from bipolar and field effect transistor [5,6] to photoelectronic devices [7]. There are also examples of active devices which were traditionally used for high frequency generation. In particular Esaki diode [8] and resonance tunneling diode [9] were proposed. Thus, 2D materials can be used for creating high frequency active element either using only 2D materials or combination of 2D and 3D materials. In submicron structures the movement of electrons is known to be close to ballistic. Therefore, adding additional active elements to the surface or changing the shape of the electrodes can strongly changes the frequency and energy characteristics of the devices. In particular, in [10, 11] it was showed that in planar structures with additional semiconductor elements placed on top of the diode side border and electrically connected to the anode of the diode, it is possible to obtain generation in a wide frequency range, including millimeter and terahertz ranges. Active element placed at side borders can influence to formation of the above-mentioned conditions both by modulating the conductivity, for example, as is the case in self-switching diodes [12], and by redistributing the charge carrier between regions of the diode having different properties similar to transfer electron device (TED). For those purposes, the using of 2D materials grown on traditional 3D semiconductors is promising, and it give a possible to combine the advantages of established 3D semiconductors with the unique properties of 2D materials.

One of these combinations can be obtained by using bulk GaN semiconductors and 2D materials, in particular transition metal dichalcogenites (TMPs) [13-21] in heterostructures of mixed sizes. That is possible to the developed planar GaN technology practically implemented in a number of devices: from light-emitting diodes to high-power electronics. Therefore, combination of GaN with 2D DPMs, such as MoS_2, is of particular importance for development of new hybrid heterostructures, including high-frequency electronics.

Theoretical studies of such heterostructures are particularly difficult, experimental research work is mandatory to reveal interfacial and electronic properties of 2D DPM/3D heterostructures and to initiate further theoretical analysis. In this section, planar diode structures containing active surface layers formed both on the basis of traditional 3D materials and using 2D TMD/3D heterostructures on the example of the MoS_2/GaN heterostructure are considered, and charge transfer between two electronic subsystems in one device is investigated.

II. MODEL

Usage of 2D materials with 3D GaN is an example of a 2D/3D structure corresponding all the general requirements for heteropairs in contact. These heterojunctions have been actively studied in the latest 5 years both experimentally and theoretically [16,18–23]. In the first works, heterojunctions between GaN−MoS_2 [18] and GaN−WSe_2 [19] are considered. The authors grew undoped GaN on 2D materials and performed high-resolution X-ray photoelectron spectroscopy to determine the position of the band gaps in these heterostructures.

In work [16], MoS_2 was grown on an n- type GaN film, initially formed on sapphire. Using the methods of atomic force microscopy with a conducting probe, it was shown that the MoS_2/GaN heterostructure electrically conducts in the direction perpendicular to the plane separating the materials through the van der Waals gap.

In [21] it was shown that heterodiodes with p-n junction p-MoS_2 − n-GaN could also be realized as a structure, in which rectification effect characteristic of ordinary diodes is observed. A number of data regarding the position of zones are currently somewhat contradictory. This fact is it is difficult to create a reliable model of the heterojunction in MoS_2/GaN. In addition, the influence of the layer formation order can change electronic properties of the semiconductor interface.

Thus, in work [21], an assumption was made regarding possible dependence of the size of the band gap on the type and level of doping. The result obtained in it indicates the formation of a contravariant heterojunction with a conduction band gap of about 0.51 eV and a significant transfer of electrons from GaN (p- type) to MoS_2. This result coincides by order of magnitude with the data obtained later in the works [22,23], where a similar conclusion is drawn as a result of the study of the structure with an n-type channel. It is also confirmed by theoretical calculations using the method of the hybrid electron functional density. In work [23] it is shown that the value of the conduction band gap for the MoS_2 – 3D GaN heterojunction depends on the number of GaN layers and monotonically decreases when going from a monolayer to a bulk semiconductor, reaching a value of 0.6 eV in the latter. It is this value used in our work.

The cross-section of the planar diode structure under study is shown in Fig.1. It consists of a conductive layer (active layer) (2) formed on a high-resistance (semi-insulating) substrate (1) with two ohmic contacts (5,6). The 2D semiconductor layer (7) is placed on top of the channel and occupies the area from the cathode to the anode contact, but not electrically connected to the n^+- region of the cathode contact (3).

To simplify the analysis, it is assumed that the monolayer contacts the metal anode contact only within the n^+- region. All metal-semiconductor contacts are assumed to be ohmic. Heavily doped contact areas (n^+) have a size of 0.16 × 0.32 μm and donor concentration of $5 \cdot 10^{23}$ m^{-3}. Thus, the active region of the diode has a length of 0.98 μm. The concentration of the active n- layer of the basic diode structure was $(1–6) \cdot 10^{22} m^{-3}$.

Synchronous Ensemble Monte Carlo was used. To analyze the processes in GaN, a three-valley model of the conduction zone was considered. It takes into account lower Γ and upper Γ_1 and M-L valleys. The lower Γ valley is described by non-parabolic electron dispersion law $E_e(k)$. All essential electron scattering mechanisms were taken into account in the calculations: acoustic phonon, polar optical phonon, impurity, piezoelectric, nonequivalent intervalley and equivalent intervalley. We also took into account piezoelectric scattering, which significant effects on kinetic characteristics both in nitrides and MoS_2. Dielectric properties of medium bordering the monolayer arising due to placing it on the surface of a bulk semiconductor are taken into account in assumption of infinitely thin layer according to [24].

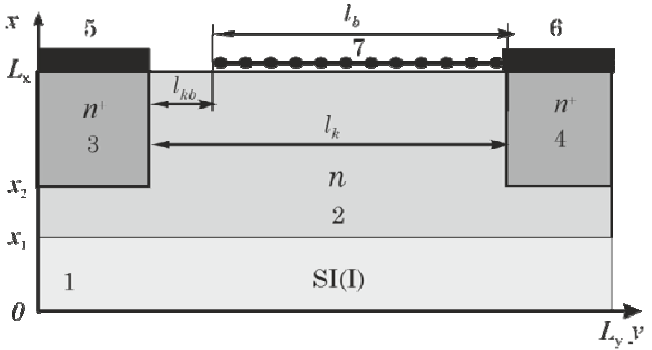


Fig. 1. Diode structure: semi-insulating substrate (1), channel (2), heavily doped contact area (n^+) (3,4), cathode (5) and anode (6) - metal contacts, MoS_2 monolayer (7).

Probability of impurity scattering is determined by using the charged impurity scattering model proposed in [25] including effect of the dielectric environment, in particular, GaN layers. The conduction zone of MoS_2 is described by parabolic lower K valley, the accompanying K' valley located between the Γ and K valleys, it lies about 200 meV above the edge of the conduction band [25]. Valleys K, K' occupation in n-type MoS_2 located in the corners of the hexagonal Brillouin zone. Due to their isotropic and parabolic nature, they can be described in a good approximation by simple parabolic zones with an effective mass of $m^*=0.48m_e$.

Two-dimensional nature of carriers leads to a constant density of states. The high density of states resulting from the large value of the effective mass of the conduction band in the K, K' valleys leads to a non-degenerate carrier distribution.

All the main scattering mechanisms characteristic of 2D materials were included in simulation. It is taken into account that in two-dimensional materials there is absence of periodicity in the direction perpendicular to the layer which eliminates splitting in the LO—TO phonon modes, and therefore influence of the LO mode on the macroscopic polarization in the monolayer can be neglected. The parameters of the materials used in the calculations are selected similarly to [26].

The main parameter that is of the greatest interest from the point of view of high-frequency applications is the value of the capture time of charge carriers in the 3D part of the diode structure into the 2D part, since such a transition is essentially equivalent to the intervalley transfer of electrons in k-space. Today, the dominant approach is to consider the 2D layer as a quantum well with unlimited depth and, considering the processes in the 2D layer. Thus, an envelope wave functions of electrons in the direction perpendicular to the 2D layer is $\psi_\perp = A\sin(k_\perp x)$, where $k_\perp = n\pi / a$, a is the width of the quantum well. The carriers can be inside quantum well both in the trapped energy state associated with the 2D semiconductor layer and above the quantum well in the state associated with the 3D semiconductor. Therefore, relationship between three-dimensional electron gas (3DEG) and two-dimensional gas (2DEG) should be considered. Similar problems were previously considered in the context of trapping electrons in quantum wells in heterostructures [26–31].

Taking into account the peculiarities of the relative position of the conduction bands in the materials in contact, the energy minimum in the 2D material corresponding to the K valley is lower than the minimum in GaN. 3D – 2D transitions become possible under the condition when the initial energy of the electron E is not less than of electron energy in 2 D-material by the amount of optical phonon energy. Therefore, the probability of 3D → 2D capture is practically equal to the total probability of completing any transition with an emitted optical phonon. Considering the non-degeneracy of the initial and final states and the dominance of electron scattering by polar optical phonons in GaN at low energies, the polar-optical phonon exchange is most probable the dominant mechanism of such transitions.

The probability of electron transitions from the initial state $\vec{k}$ with energy E_i in the 3D material to any other state

$\vec{k'}$ with energy E_i due to the absorption or emission of a phonon with energy $\hbar\omega_q$ is reduced to the determination of the coupling parameter C_q for the given mechanism and the overlap integral $I^2(\vec{k},\vec{k'},q_x)$ and the calculation of the integral (1) for all possible states $\vec{k'}$ in a 2D semiconductor:

$$W_{if}^{\pm} = A\int C_q^2 I^2 \left(N_{qb} + \frac{1}{2} \pm \frac{1}{2}\right)\delta(E_{\vec{k'}} - E_{\vec{k}} \pm \hbar\omega_{qb})d\vec{k'}, \quad (1)$$

where $A = (4\pi\rho_S\omega_{qb})^{-1}$, ρ_S - surface density of MoS_2, N_{qb} - phonon occupation number. The probability of a reverse transition from the initial state with energy in 2D material to any other state with energy in 2D material is determined in a similar way. In both cases, it is assumed that transitions occur as a result of interaction with bulk optical modes of GaN.

The definition of integral (1) over all final states is carried out by integration over the possible polar angles to obtain the expressions for the probabilities as an integral over interval of value of transmitted moment q. The value of the emitted (absorbed) phonon momentum as a result of scattering is determined using the Neumann procedure using probability density function. Taking into account the parabolic law of dispersion in GaN and MoS_2, momentum values and final energy states are determined from the conservation energy law:

$$k_{2-D}^2 = \frac{2m^*_{2D}}{\hbar^2}\left(\left(E - \Delta E_C \pm \hbar\omega_{LO}\right) = \right.$$
$$= \frac{m^*_{2D}}{m^*_{3D}}k_{\parallel}^2 + \frac{2m^*_{2D}}{\hbar^2}\left(\frac{\hbar^2 k_x^2}{2m^*_{3D}} - \Delta E_C \pm \eta\hbar\omega_{LO}\right), \quad (2)$$

$$p_{3-D}^2 = \frac{m_{3D}}{m_{2D}}(E_i \pm \hbar\omega_{LO} + \Delta E_C). \quad (3)$$

The angle between the initial and final wave vectors is determined from the law of momentum conservation. The limitation caused by the two-dimensional model is related to the fact that the width of the monolayer is assumed to be equal to the width of the diode, while the nature of the movement of charge carriers under the monolayer is a three-dimensional process and depends on the distribution of the electric potential in the transverse direction, which, due to the small areas of the monolayer, can be significantly uneven.

All contacts of metal to a semiconductor are suggested to be ohmic ones. Values of electrostatic potential involved contact different potential due to difference material at the cathode and anode were fixed. To obtain the electrostatic potential distribution the 2D Poisson equation was solved by using of geometric full multigrid (FMG) method. Sampling the particle motion is realized at a very small-time interval of $\Delta t = 10^{-17}$ s. The mathematical model details are accorded to [32]. Material parameters of GaN and MoS_2 are corresponded to [33] and [26] respectively.

III. Results and Discussion

The characteristics of the diodes were considered in t voltage range of 0 – 8 V. This guaranteed limitation of the energy of the electrons and their localization in the parabolic Γ- valley of GaN, which corresponds to the calculation model. The cases of n-GaN – undoped MoS_2 transitions and n-GaN – n-MoS_2 transitions are considered. Additionally, the situation when the diode contains a lightly doped layer located between the n^+- contacts, which separates the main part of the diode from the monolayer, is considered (Fig.2,3).

As it can be seen from the dependences, the presence of a monolayer in the considered structure has little effect on the drift conditions of charge carriers along the diode channel. The area of space charge that occurs at the GaN–MoS_2 separation boundary does not exceed 0.05 μm in size. Since the probability of scattering of an electron by a polar optical phonon has a weak dependence on the energy of the electron, the capture of charge carriers in the 2D- layer occurs along the entire length of the monolayer Fig.4.

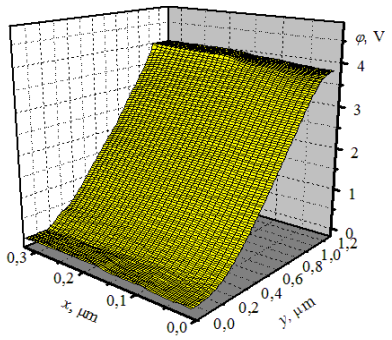
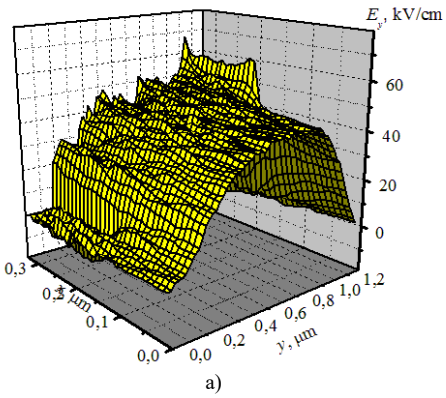
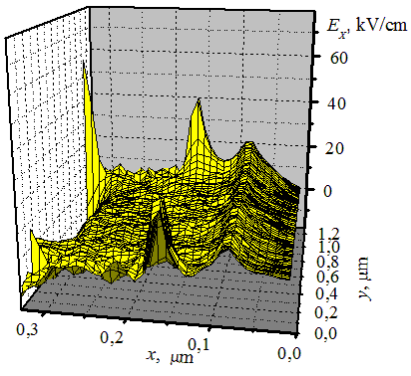


Fig. 2. Distribution of electrostatic potential in a diode, $N_S = 0$, $l_{ib} =$ 0.16 μm.



a)



b)

Fig. 3. Distribution of E_y a) and E_x b) - components of electric field intensity, $N_S = 0$, $l_{ib} = 0.16$ μm.

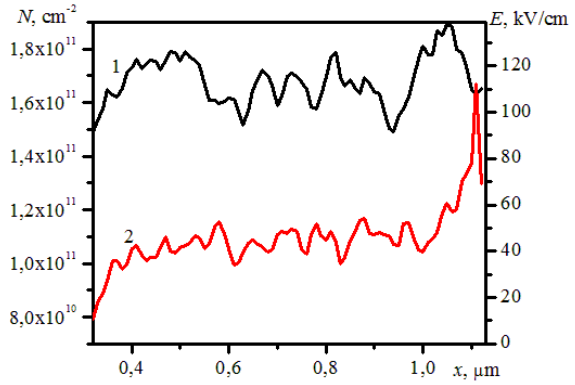


Fig. 4. Static distribution of surface electron concentration (1) and electric field strength (E_y) (2) in a monolayer, $N_S = 0$, $l_{kb} = 0{,}16$ μm, $U = 0$ V.

Due to presence of a potential barrier between the monolayer and the bulk semiconductor, the space charge is somewhat higher in the contact region and increases the electric field in the region of the 2D MoS_2 – n^+- GaN- anode interface. The main mechanism limiting 3D → 2D transitions is the formation of a potential barrier.

In Fig.5 the dependence of the current density on the voltage for diodes based on GaN with 2D MoS_2 – 3D GaN heterojunctions, which had different doping levels in the monolayer, are shown. The figure also shows the dependence of the current density on the voltage for a conventional (without MoS_2 –layer) GaN- based planar diode.

Dependence 5 was obtained for the diode containing a weakly doped layer 80 nm thick, which was located between n^+- contacts and separated the main part of the diode from the monolayer. It can be seen from the given dependences that the presence of a heterojunction reduces the amount of current flowing through the diode, but practically does not change the qualitative current-voltage dependence. Also, the presence of heterojunction does not affect the qualitative behavior of the introduction of a weakly doped layer, which only reduces the conductivity of the channel. Under condition that the value of the band gap between the contacting materials does not change, the conductivity of the monolayer has a weak effect on the current of the diode structure.

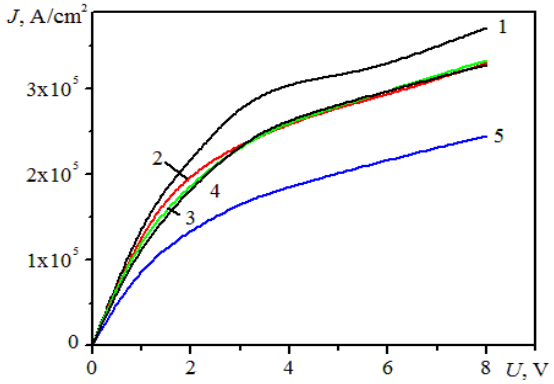


Fig 5. Dependence of current density on voltage for diodes based on GaN without a heterolayer and with a heterolayer with a thickness of 0.8 μm (l_{kb}=0,16 μm): 1 – diode without heterojunction; 2-5 diode with 2D-MoS_2 – 3D GaN heterojunction: 2– $N_S = 0$; 3, 5– $N_S = 10^{11}$ cm^{-2}; 4– $N_S = 10^{12}$ cm^{-2}.

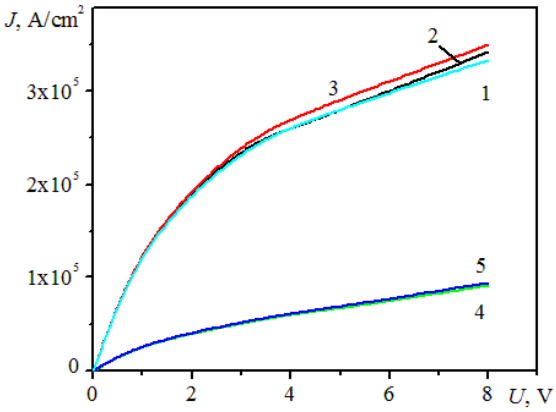


Fig. 6. Dependence of current density on voltage for diodes with 2D-MoS_2 – 3D GaN heterojunction, donor concentration $N_S = 10^{11}$ cm^{-2}: 1 – $l_b = 0.8$ μm; 2,4 – $l_b = 0.64$ μm; 3,5 – $l_b = 0.48$ μm.

The biggest differences are observed in the voltage range of 0–2.5 V and are related to the dependence of the phonon scattering probability on energy.

Fig. 6 shows dependences of the current density on the voltage for GaN-based diodes with 2D-MoS_2 – 3D GaN heterojunctions with different monolayer lengths. The main differences are observed at high voltages, which is mainly due to the effect of the space charge in the diode channel. Decreasing the carrier's concentration in the channel weakens this effect. Differences in dependencies are not observed.

IV. Conclusions

Using the Monte Carlo method, simulation of electronic processes in planar diodes containing a 2D–3D semiconductor heterojunction has been carried out.

The static characteristics of planar diodes with a 2D MoS_2 – 3D GaN heterojunction were obtained within the framework of the proposed model. It was shown that the arrangement of the monolayer along the diode channel leads to a decrease in the current through the diode but does not qualitatively change the current- voltage dependence.

Our simulation shows that the electron transition process time between 3D and 2D regions is about 10 ps on average. Therefore, considered structures can be investigate further for their possible high frequency application.

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