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REGULAR ARTICLE

Self–Heating Effect in Planar GaN Diode with 2D- *h*-BN - Layer

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In this research, we have studied a self-heating effect in hybrid 2D-3D heterostructure diode, considering planar GaN-based structure of 1280 nm with *n*-type channel and donor concentration of $6 \cdot 10^{17}$ cm^{-3}. Two type *c*-plane substrate-based sapphire and GaN are considered in order to investigate heating effects in diode channel. Monolayer hexagonal boron nitride (*h*-BN) on the top of canal is considered as an element for thermal control of the diode. The model of a heating based on macroscopic thermal parameters of materials is used. The simulation of diode operation was carried out using the Ensemble Monte Carlo Technique self-consistently with numerical solving of system of heat equations by full multigrid (FMG) method. Transport properties of diode is considered under condition of high electric fields and impact ionization. Characteristics of the diode with both *h*-BN monolayer and without one were obtained at DC applied voltage.

A temperature distribution in diode is obtained with account of thermal boundary resistance at each interface, considering voltage range of 0-20 V. In strong electric field in anode, the heating rises maximal temperature in channel diode up to over 600 K. The *h*-BN was found to affect the temperature magnitudes and their redistribution in diode channel. Temperature decrease can achieve 3 % and increase in case of high temperature region. Role *h*-BN monolayer as a factor avoiding formation of localized overheating of a device is demonstrated. It is shown that, *h*-BN monolayer is effective in diode using the substrate with low thermal conductivity and can be applied for semiconductor devices with length of several micrometers.

Keywords: Monolayer, GaN, Heterostructure, Substrate, Temperature, Electric field strength, Self-heating effect, Thermal conductivity, Thermal boundary conductance, Heat equation, Impact ionization.

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1. INTRODUCTION

Two-dimensional (2D) materials attract a great attention due to their excellent properties [1]. For example, ultra-high room-temperature thermal conductivity of above 2000 W/(m·K) have been observed in graphene for the first time. Theoretical and experimental study shows that the phenomenon is connected to acoustic phonons due to the presence of strong scattering process in graphene and its derivatives [2]. These results have stimulated great interest in exploring other emerging 2D materials. Among them, atomic thin h-BN is attractive. Unlike zero band-gap graphene, it has 5.8 eV band-gap, and can been considered the top ranked candidate for the dielectric material for next-generation electronic devices [3]. An in-plane thermal conductivity of one layer (1-L) h-BN as high as 585 W/(m·K) at room temperature have been obtained experimentally in [4]. Experimental results of Raman-deduced average thermal conductivity for 1-L BN of 751 W/m·K were obtained at room temperature, in [3]. The thermal conductivity of higher than 800 W/(m·K) is reported in [5].

Thus, waste heat can spread quickly laterally through a large area, avoiding formation of localized overheating of a device [6]. This approach is expected to be effective in heterostructures composed of distinct 2D materials. Hence, it can also be used in combination with *h*-BN with 3D – material in the so-called hybrid heterostructures with mixed sizes. One of these combinations can be obtained by using bulk GaN semiconductors and 2D materials in van der Waals heterostructures [7]. Due to the developed planar GaN technology 2D/3D heterostructures have already been proposed and practically realized, for example, by a combination of GaN with 2D transition metal dichalcogenides (TMPs), such as MoS_2 [8]. A number of new hybrid heterostructures from light-emitting diodes to high-power electronics has already been practically implemented [9]. Theoretical studies of such heterostructures from the first principles are difficult, and cannot be used in large structures. At the same time, results of experimental determination of thermal parameters of h-BN suitable for estimation of its usage for device design are known in the form of thermal conductivity value [3], and can be implicated to thermal characteristics device contained *h*-BN layer.

The objective of this paper is to consider the usage a 1-L *h*-BN layer in planar GaN diode structures under a strong electric field and impact ionization (II) by accounting self-heating effect in them.

2. STRUCTURE AND SIMULATION

Cross-section of a 2D/3D heterostructure diode is shown in Fig. 1. Diode represents of GaN-based n^+-n-n^+- type structure with length of 1.28 μm. Donor con-

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centration is $6 \cdot 10^{16}$ cm^{-3} and 10^{19} cm^{-3} in n region and highly n^+ regions respectively. A diode thickness L_x is 0.32 µm. An active diode length l_a is about 1 µm.

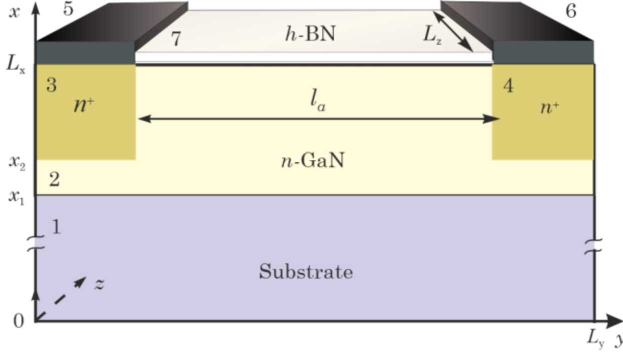


Fig. 1 – Diode structure: low conductivity substrate (1), n-type diode channel (2), high doped contact region (3,4), metal contacts (5,6), h-BN- layer (7)

Contacts are considered to be ohmic. The n^+-region's size is 0.16 × 0.32 µm. The h-BN layer is supposed to place on the top of the diode channel between contacts connecting with them. The thermal properties of 1-L h-BN were accounted by using a classical definition. The in-plane thermal conductivity of $k(T)$ is used as a parameter. For estimate of $k(T)$, the experiment results obtained from assumption of h-BN monolayer's sickness is d (0.52 nm) were taken into accounted [3]. The use of simple relations between heat flux and temperature in experiment confirms the correctness of this approach [3]. In fact, $k(T)$ is a characteristic of macroscopic layers and can be used to estimate of their thermal properties. Heat transfer between h-BN and GaN is known to be determined by particle scattering at interfaces. Surrounding h-BN film acts as diffuse phonon absorber and provides a boundary condition that resembles phonon scattering on the boundaries of a GaN with roughness. For this reason, the efficiency of heat flow, both at h-BN-GaN interfaces, and metal-GaN interfaces, were described by the thermal boundary conductance (TBC) h_B:

$$q_S = h_B(T - T_S)\,, \tag{1}$$

where q_s is a heat flux across two material interface; T_S and T are temperatures of h-BN, GaN respectively.

Thus, under assumption of invariable temperature across x – direction in 1-L (See Fig. 1), consider an element of monolayer with volume $\Delta V = d\Delta y L_z$. Then, at $\Delta y \to 0$ for modeled 2D – domain corresponding, the energy balance under non-steady state conditions has the form:

$$c_S \frac{\partial T_S}{\partial t} = \frac{\partial}{\partial y}\left[k_S \frac{dT_S}{dy}\right] - a_B(T_S - T) - a_A(T_S)(T_S - T_A))\,, \tag{2}$$

here c_S is a volumetric heat capacity of BN [10]; T_A is the ambient temperature; $a_B = h_B/d$, $a_A = (h_S + \varepsilon\Phi(T_S))/d$, h_S is heat transfer coefficient of convective between material and the ambient, ε is a radiating ability of 1-L.

The free fly length associated with phonon scattering in nitride compounds in practice is less than 100 nm. This fact enabled us to neglect scale effect connected with heating and to calculate temperature distribution in GaN using the heat equation:

$$c\frac{\partial T(r,t)}{\partial t} = \nabla \cdot \left[k \nabla T(r,t)\right] + F(r,t) \tag{3}$$

here k is the thermal conductivity, and c is the lattice heat capacity, $F(r,t)$ is defined as a form [11]:

$$F = F_0 \sum\left(\hbar\omega_{ems} - \hbar\omega_{abs} + \Delta E_{II}\right), \tag{4}$$

here $\hbar\omega_{ems}$, $\hbar\omega_{abs}$ are phonon energy at phonon emission and phonon absorption respectively, ΔE_{II} is absorbed energy by lattice at II process, F_0 is a constant depending on parameter of numerical model and device doping. Temperature dependence of $k(T)$ for used materials is taken on form [12]:

$$k(T) = k_{300K}\left(T/300\right)^n\,, \tag{5}$$

here k_{300K} is thermal conductivity at 300 K that to be sickness depended [13]. Thermal parameters of material corresponded to GaN of 320 nm are given in Table1.

Table 1 – Thermal parameters

Parameter	h-BN	GaN	Al_2O_3
k_{300K},W/(K·m)	800[5]	80;130[13]	40[14]
n	0	– 0,43[12]	–
c, J/(m^3·K)	$1.6 \cdot 10^6$[10]	$3 \cdot 10^6$ [12]	$3 \cdot 10^6$
h_A, W/(K· m^2)	20	20	–
h_B, W/(K· m^2)	$3.5 \cdot 10^7$[15]	–	10^7[16]

Here, the TBC h_B is given for the interface between material and GaN. Ohmic contact is suggested to be gold with a titanium adhesion layer. The TBC for metal-GaN interfaces is $2 \cdot 10^8$ W/(K·m^2) [17]. The parameter h_S is considered to be the same for GaN and as h-BN, and it was taken equal to 20 W/(K·m^2).

The lattice heat capacity is considered to be independent on temperature both for h- BN, and diode materials.

The isothermal boundary condition (300 K) is performed at $x = 0$ (a perfect heat sink). The adiabatic thermal conditions are applied to left ($y = 0$) and right ($y = L_y$) boundary.

To simulate the non-equilibrium charge transport, the synchronous Ensemble Monte Carlo approach was used [18] self-consistently with Poisson's equation and system of heat equations (2) and (3). The equations were solved numerically by full multigrid (FMG) method [19].

Three lower nonparabolic valleys of conductivity band (Γ, Γ$_1$ and M–L valleys) were considered. Bias voltage is suggested not to be large enough to case significate II in diode. The valence band is accounted for by heavy holes zone only. Other simulation details and parameters of GaN are applied according to [18].

Effect of temperature on diode operation was taken into account by temperature dependences of scattering parameters, energy gap, and threshold energy of II.

3. RESULT AND DISCUDION

The main difficulty in obtaining the characteristics of diodes, taking into account self-heating, is long time to achieve the steady state temperature in the device. The time step required for the correct use of the Monte Carlo method has an upper limit due to the high intensity of scattering in GaN and is taken $2 \cdot 10^{-16}$ s. For this reason, the analysis of the structure under self-heating was limited by simulation time $t_{sim} < 25$ ns. Electric field distribution in diode channel is shown in Fig. 2.

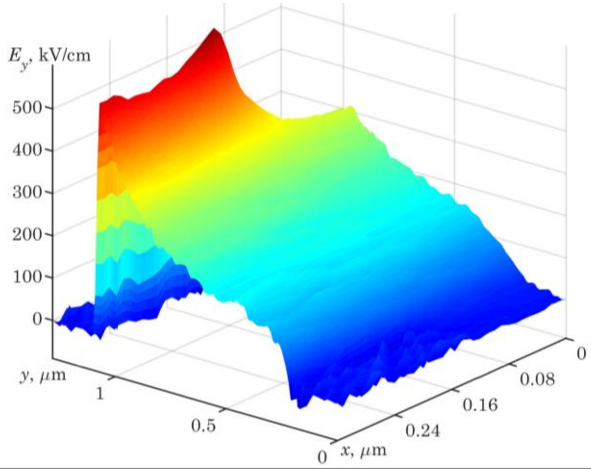
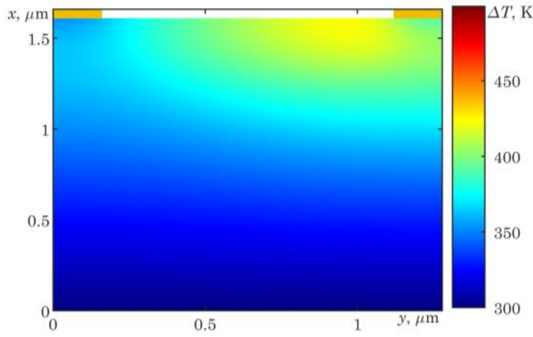
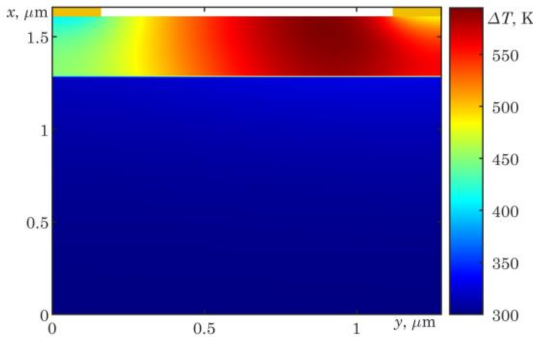


Fig. 2 – Distribution of y-component of electric field in the diode channel of the diode (GaN on sapphire substrate) with h-BN monolayer, $U = 20$ V



a)



b)

Fig. 3 – Temperature distribution in the GaN diode at $U = 20$ V for two substrate ($t_{sim} = 25$ ns): a) GaN; b) sapphire

In case of high doping concentration in short diode, the non-uniform carrier distribution leads to growing electric field from cathode to anode. Thus, kinetic electron energy of electron reaches maximum at the anode contact. It is the region with intensive scattering electron on deformation potential of optic phonon, and impact ionization and overheating effects are possible.

Temperature distributions in diode for two difference types of substrate are shown in Fig. 3.

This is typical for GaN device. For example, in FET high electric fields also can result in significant hot-spots localized near the drain side of the gate contact. The temperature maximum in all considered cases corresponds to top surface of channel at anode.

As can be seen from Fig. 3, the thermal properties of substrate are confirmed to affect the channel temperature rise. The temperature of the sapphire substrate is differed from that of channel one. That results from both low thermal boundary conduction of GaN/sapphire interface and lower thermal conductivity of sapphire.

Dependences of current density and maximal temperature in diodes on applied bias voltage are shown in Fig. 4.

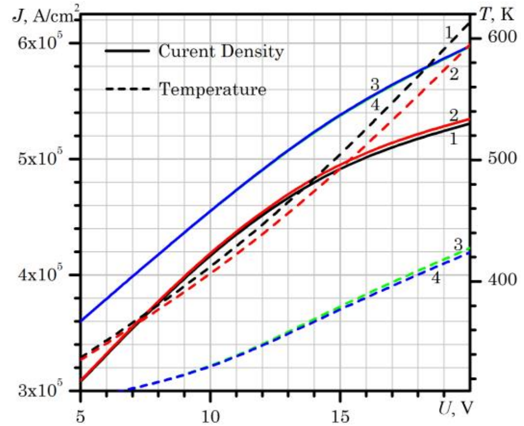


Fig. 4 – Current density and maximal temperature in channel as a function of bias voltage ($t_{sim} = 25$ ns): 1, 5 – GaN substrate without h-BN: 2, 6 – GaN substrate with h-BN: 3, 7 – sapphire substrate without h-BN: 4, 8 – sapphire substrate with h-BN

The temperature magnitude depends strongly on bias voltage. In case of h-BN, the temperature decreases. Simulation results for $t_{sim} = 25$ ns demonstrate that maximal temperature is more than 614 K in case of GaN channel on sapphire substrate without h-BN. In case of 1-L h-BN, the temperature digresses to 595 K. In fact, the highest temperature value in diode channel the more temperature decreasing due using 1-L h-BN can be obtained. At the same time, the current density change is weakly. Temperature distribution in the top layers of GaN surfaces in diode on sapphire substrate at $U = 20$ V ($t_{sim} = 25$ ns) is shown in Fig. 5.

Here, the temperature in 1-L, and GaN surface in diode 1-L and with 1-L are presented. The most deference in diodes temperature is achieved in anode, corresponding to maximal heating region. Thus, the proposed way to temperature decrease is most effective when localization of electric field within the device leads to large hot-spots. The most effective temperature decrease is up to 3 %.

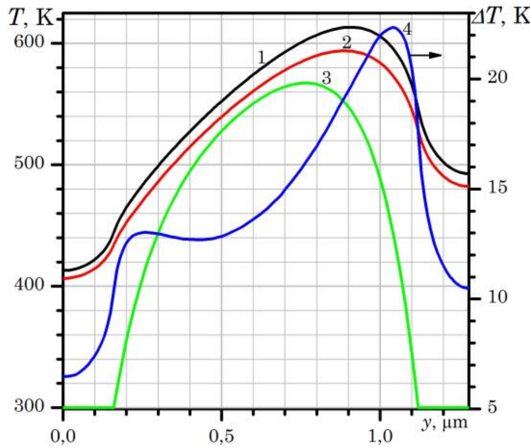


Fig. 5 – Temperature distribution on the top layers of diodes: 1 – GaN channel without SL *h*-BN; 2 – GaN channel with SL *h*-BN; 3 – SL *h*-BN; 4 - temperature difference

Due to more low study-state temperature, under the same applied voltage, effect of *h*-BN in diode with GaN substrate is weaker. However, temperature conductivity of sink GaN is known to drop to 20 W/(m·K) if it's length is less than 40 nm [13]. In this case, fraction heat energy dissipating throw top surface increases, and effect of *h*-BN layer on the diode temperature will be appreciable.

4. CONCLUSIONS

We present the result of Monte Carlo simulation of planar diode based on hybrid 2D-BN/3D-GaN- heterostructure diodes with account of self-heating effects in them.

Unique temperature properties of 1-L *h*-BN are treated in relation to the problem to obtain an operation stability of micrometer device under self- heating effect in strong electric fields and significant current density in them.

Our investigation demonstrates that using 1-L h-BN for temperature control in nitride-based diode with length of few micrometers is possible.

Diode characteristics with account and without account of 1-L on top surface of diode is obtained. Such an analysis applied to GaN devices indicates that the effects of temperature decrease due to presence of *h*-BN 1-L should be quite noticeable in the devices when using substrates with low temperature conductivity like sapphire.

Scale effects was partially taken into account in the thermal conductivity of GaN. However, they may be noticeable already at size of several micrometer [13].

It is clear that for the device with the size of the order of free fly phonon length the modeling of thermal transport becomes increasingly complicated.

The proposed method to analyze thermal process on the base on Monte Carlo simulation is suitable for micron size device because of high accuracy and most effective FMG to find temperature distribution in many-layer micron size device with account of thermal boundary conductance across interfaces.

1-L *h*-BN can be incorporated into the device in other way. It can be considered as tunable dielectric material able to change both thermal and electric properties of the device. For example, it can be applied in hybrid 2D-3D diodes with lateral electron transport in heterolayers [8], and also in high frequency and power devices for enhancing their characteristics depending on temperature [20].

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Самонагрівання у планарному GaN діоді з 2D-h-BN- шаром

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Проведено дослідження ефекту саморозігріву у гібридних 2D-3D гетероструктурних діодах. Розглядається планарна структура на основі GaN довжиною 1280 нм з каналом *n*-типу та концентрацією донорів $6 \cdot 10^{17}$ см$^{-3}$. Для дослідження ефектів нагрівання в діодному каналі розглянуто підкладку двох типів: з орієнтацією у *c*-площині на основі сапфіру та GaN. Моношар гексагонального нітриду бору (*h*-BN) на поверхні каналу розглядається як елемент для теплового контролю діода. Використовується модель нагріву на основі макроскопічних теплових параметрів матеріалів. Моделювання роботи діода проводилося з використанням багаточастинкового методу Монте-Карло самоузгоджено з числовим розв'язанням системи рівнянь теплопровідності з використанням повного багатосіткового методу (ПБМ). Транспортні властивості діода розглядаються в умовах дії сильних електричних полів і ударної іонізації. Характеристики діода з моношаром *h*-BN і без нього отримано за постійної прикладеної напруги. Розподіл температури в діоді отримано з урахуванням теплового граничного опору на кожній із меж поділу. Розглядається діапазон напруг 0-20 В. Показано, що в анодній частині діода формується сильне електричне поле, що призводить до його нагрівання. Підвищення максимальної температури в каналі діода становить понад 550 К. Встановлено, що *h*-BN впливає як на величину температури, так і на її перерозподіл у каналі діода. Зниження температури може досягати 3 % і збільшується у випадку високотемпературної області. Продемонстровано роль моношару *h*-BN як фактора, що запобігає утворенню локалізованого перегріву пристрою. Показано, що моношар *h*-BN можна ефективно використовувати в діодах, які мають підкладку з низькою теплопровідністю в напівпровідникових приладах довжиною кілька мікрометрів.

Ключові слова: Моношар, GaN, Гетероструктура, Підкладка, Температура, Напруженість електричного поля, Ефект самонагрівання, Теплопровідність, Гранична теплова провідність, Рівняння теплопровідності, Ударна іонізація.