JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. 18 No 1, 01026(5pp) (2026)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том 18 № 1, 01026(5cc) (2026)

OPEN ACCESS

REGULAR ARTICLE

Oscillations in GaN Diode with 2D-h-BN – Layer

V.O. Zozulia*, O.V. Botsula, Y.S. Khodachok, K.H. Prykhodko, L.V. Sichevska

V.N. Karazin Kharkiv National University, 61077 Kharkiv, Ukraine

(Received 20 December 2025; revised manuscript received 15 February 2026; published online 25 February 2026)

In this research, we have investigated the operation of a hybrid 2D-3D heterostructure diode in the Gunn-like oscillation mode. The diode is represented as a GaN-based structure containing *n*-type channel on a sapphire substrate with the hexagonal boron nitride (h-BN) monolayer on the top. The simulation of the diode operation has been carried out by using the ensemble Monte Carlo technique self-consistently with a numerical solution of system heat equations. The model of heating based on macroscopic thermal parameters of materials has been used. Diode length is assumed to be about 1 μm and the donor concentration is $0.6{\cdot}10^{23}$ – 10^{23} m^{-3}. Direct current and oscillation characteristic of diodes with and without the h-BN monolayer have been compared. Maximal oscillating efficiency has been estimated in the possible bias range taking into account impact ionization and heating effect condition.

Our simulation shows that microwave oscillation in the n^+-n-n^+ GaN diode is limited by impact ionization and self- heating and depend upon the bias and doping concentration. Temperature distributions in the diode have been obtained. With the higher concentration the oscillation can be fully suppressed by both impact ionization and heating. There is a narrow bias range where the oscillation appears. Adding the h-BN monolayer on the top of the diode surface can decrease a local overheating effect. It has been demonstrated that presence of h-BN affects the temperature magnitude and redistribution in the transit region of the diode. The frequency range for this case is narrower and the maxi-mal efficiency is five times lower in comparison with case when the diode was not affected by impact ionization and temperature. In several cases of high doping, the microwave oscillations appear only in the diode with the h-BN monolayer.

Keywords: Monolayer, GaN, Heterostructure, Substrate, Temperature, Electric field strength, Self-heating effect, Impact ionization, Oscillation, Oscillation efficiency, Frequency range.

DOI: 10.21272/jnep.18(1).01026 PACS numbers: 85.30.Fg, 73.40.Kp, 73.40. – c

1. INTRODUCTION

The GaN-based Gunn diode is expected to produce a higher frequency and higher power capability in comparison with current GaAs devices. The maximum frequencies that GaN-diode can produce are estimated to be higher than 700 GHz. However, producing an oscillation mode in a GaN-based Gunn diode remains a difficult task. One of the basic problems is self-heating. The small thermal conductivity of sapphire substrates, which are widely used for the growth of GaN, makes the implementation of heat sinks difficult. Consequently, it leads to high dc losses and reduced reliability.

The local thermal control of device can be substantially improved by forming additional heat-escaping top-surface heat spreaders.

Two-dimensional (2D) materials attract great attention due to their unique properties, especially thermal and conductive ones. Thus, ultra-high temperature conductivity for graphene is above 2000 W/(m·K).

Both Few-Layer graphene (FLG) and Single-layer graphene (SLG) films are shown to be effective heat spreaders [1, 2]. Their advantage is relatively small thermal boundary resistance (TBR) between interface of those material and various substrates. However, both FLG and SLG are high conductivity materials. Unlike zero band-gap graphene, the hexagonal boron nitride (h-BN) monolayer represents wide band–gap semiconductors (E_g = 5.8 eV), and can been considered as a dielectric material for next-generation electronic devices [3]. The temperature conductivity higher than 800 W/(m·K) has been observed experimentally for h-BN [4].

Thus, by using h-BN heat can be spread laterally through a large area, avoiding localized overheating of the device [5].

h-BN can used both in the heterostructures composed of a 2D materials and, in combination with a 3D-material, in the so-called hybrid heterostructures of mixed sizes [8]. Bulk GaN is known to form 2D/3D heterostructures with many 2D materials including metal dichalcogenides (TMPs) [7], and h-BN [8]. Taking into account the widespread usage of III-nitride for development of solid state electronic and optoelectronic

* Correspondence e-mail: v.zozulia@karazin.ua

devices associated with the problem of overheating, the possible application of h-BN to decrease temperature in a device can be beneficial. The application of h-BN in such a manner has been considered in [9] for the planar GaN-based diode. It has been shown that the h-BN layer on the top of a diode channel leads to decreasing a maximum temperature in the diode [9].

The aim of this paper is to consider the usage the h-BN monolayer (1-L) in the planar GaN-based diode to obtain a microwave oscillation.

2. STRUCTURE AND SIMULATION

The diode configuration is suggested to be a substrate with finite-thickness, and a fixed temperature at its bottom boundary is assumed to be 300 K. The sapphire substrate thickness is assumed to be 1.28 μm, and its length is equal to the diode length.

The device structure is the same as considered in [9], and their cross section is shown in Fig. 1.

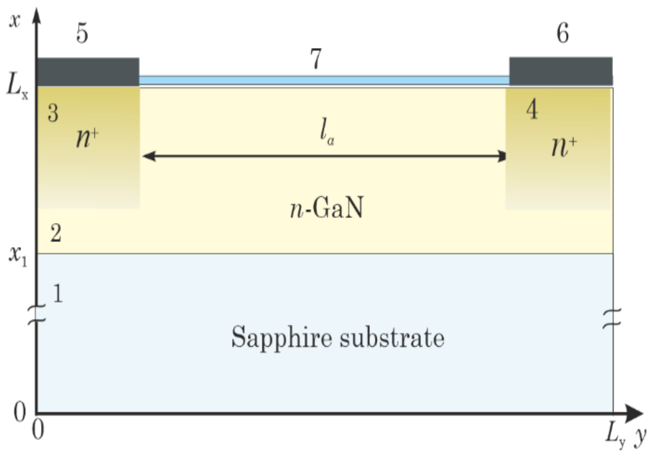

Fig. 1 – Diode structure: substrate (1), n-type diode channel (2), high doped contact region (3, 4), metal contacts (5, 6), h-BN-layer (7); l_a – transit region length

The uniformly doped n-type transit region with the on 1 micron is assumed to be sandwiched between two n+ regions. The donor concentration has been set with consideration for possible appearance of oscillations in accordance with Kremer criteria for GaN-based Gunn diodes (from 6×10^{22} m^{-3} to 2×10^{23} m^{-3}). The contacts are considered to be ohmic, and the contact regions of 0.16 μm × 0.32 μm are doped at 1×10^{25} m^{-3}. The total length is 1.28 μm and L_x is 0.64 μm (Fig. 1).

The h-BN layer is placed on the top of the diode channel contacting both the cathode and anode. The ohmic contact is suggested to be gold with a titanium adhesion layer [10].

The thermal properties of 1-L h-BN have been accounted by using a classical definition. The heat properties of the system are considered in the framework of the model described in [9]. Efficiency of heat flow at all interfaces between different materials including metal-GaN interfaces has been described in term of the thermal boundary conductance (TBC). All thermal material parameters are in accordance with [9].

To simulate the non-equilibrium charge transport during the high-frequency operation, the synchronous ensemble Monte Carlo approach has been used [11] self-consistently with the analysis of diode heating.

The three lower non-parabolic valleys of a conductivity band (Γ, Γ_1 and M–L valleys) have been considered. The valence band is accounted by the heavy holes zone only.

The zone parameters of GaN and actual scattering mechanisms for electrons and holes are taken into account according to [11]. Other simulation details and parameters of GaN are applied according to [9].

The effect of temperature on diode operation is represented by the temperature dependence of the scattering parameters, energy gap, and threshold energy of impact ionization.

The field-adjusting timestep is 0.5 *fs*. About 100,000 superparticles have been used in each simulation. The heating time has been limited by the simulation time $t_{sim} < 100$ ns.

3. RESULT AND DISCUDION

The experimental data of generation in GaN have not been thoroughly studied. An important exception is the case of a GaN-diode on GaN substrates considered in [12]. Therefore, in our study we have followed the simulation results obtained for a GaN-based diode with the length of about 1 micron, that has been formed on a sapphire substrate.

The presented results have been obtained with taking into account both impact ionization effect and self-heating. The frequency and energy characteristics of the GaN-based diode have been acquired under assumption that the diode is placed in a single-circuit resonator. The voltage waveform applied to the diode is considered to be in form $U(t) = U_0 + U_1 \sin 2\pi f t$, where f is the resonator frequency; U_1 is the amplitude of the first voltage harmonic: U_0 is the dc bias voltage. The oscillation efficiency is determined as the alternative power P to DC power ratio $\eta = P / P_0$. The maximal oscillator efficiency is estimated by optimizing U_0 and U_1 magnitudes. In this way we obtain the maximal oscillation efficiency $\eta_{\max}$ at a fixed resonator frequency.

In our case the maximal oscillation efficiency corresponds to the bias close to $U_0 = 35$ V. However, we must take into account the fact that impact ionization and heating can significantly affect the transport of carriers in a diode. The dependence of the current density on dc bias applied to a diode in case of different doping of the transit region is demonstrated in Fig. 3.

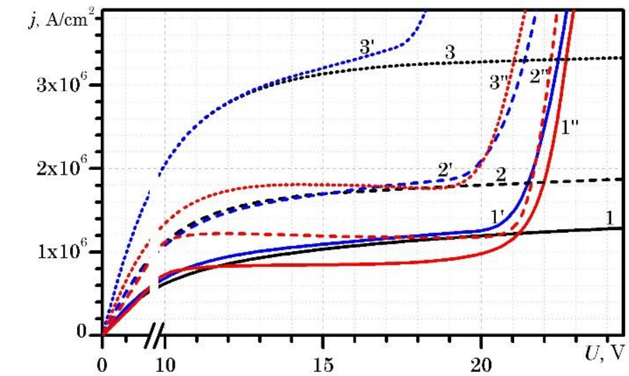

Fig. 2 – Dependence current density on voltage bias 1, 1',1" – $N_d = 6 \times 10^{16}$ cm^{-3}, 2, 2', 2" – $N_d = 10^{17}$ cm^{-3}, 3, 3', 3" – $N_d = 2 \times 10^{17}$ cm^{-3}: 1-3 – w/o II and w/o self-heating; 1'-3' – with II and w/o self-heating; 1"-3" – with II, with self-heating

The three types of dependences, namely, the diode under effects of II and heating, the diode under effects of II only, and the diode without effects of II and heating have been considered. It follows that presence of II leads to narrowing of the voltage range that can be used for generation. Heating, which will be significant in the case of higher doping concentration, will only slightly reduce the effect of impact ionization, while simultaneously reducing electron mobility and current density. This leads to a noticeable decrease in the oscillation efficiency or possible disappearance of the oscillations.

To evaluate the contribution of those mechanisms the bias dependence efficiencies at several frequencies has been defined (Fig. 3) for abovementioned cases both with and without h-BN. As expected, the maximal bias voltage corresponding to stable generation is reduced significantly. There is a narrow bias range where the oscillation appears. The lower value is limited by self-heating effect, but the upper value by both II and self-heating simultaneously.

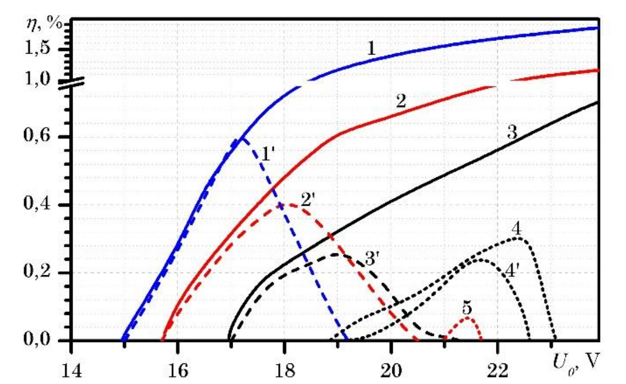

Fig. 3 – Voltage dependence of oscillation efficiency at $f = 250$ GHz for different doping concentration: 1, 1' –$N_d = 2 \times 10^{23}$ m^{-3}; 2, 2', 5 – $N_d = 10^{23}$ m^{-3}; 3, 3', 4, 4' – $N_d = 6 \times 10^{22}$ m^{-3}; 1-3 – w/o II and self-heating; 1'-3' – with II and w/o self-heating; 4, 5 – with SL h-BN, with II and self-heating; 4' – w/o SL h-BN, with II and self-heating

The changes in temperature due to the h-BN monolayer depend upon the local temperature distribution. The temperature along the diode transit region at the diode surface for the cases of a diode with and without monolayer, is shown in Figs. 4 and 5.

All the results have been obtained per the simulation time (t_{sim}) of 100 ns at the different diode bias. For the n^+-n-n^+ diode the maximal magnitude of an electric field is located at the end of the transit region, that can lead to significant overheating. In the above-determined bias region the maximal temperature can rise above 900ºC near anode. In case of diodes with h-BN the maximal temperature can be 150 degrees lower. The difference can be seen as insignificant, but the decrease in temperature can be important factor for diode-anode contact, preventing the contact destruction. For example, the ohmic contact between Ti/Au and GaN can be stable during the short-term heat treatment at 900ºC [13]. But this temperature can be lower in case of other contacts. The frequency dependence $\eta_{\max}$ obtained as a result of the Monte Carlo modeling for the diode with different donor concentrations in the channel region with the length of approximately 1 μm, as well as similar results from several other sources, are shown in Fig. 2 for the diode without the h-BN monolayer.

For the given diode length (without effects of II and self-hearing) the oscillation efficiency is about 1-1.5 % and the corresponding oscillation frequency is 220-250 GHz depending on doping and the size of diodes.

Under effects of II, the criterion for generation stability is $at_0 / I_0 > 0.015$, where a is the slope coefficient of linear regression of the current density–time dependence, t_0 is the characteristic time (100 ns in calculation); I_0 is the average current density. The frequency range for is almost the same and the maximal efficiency is five times lower in comparison with case when the diode without self-heating and II. At higher doping concentration (1-2 10^{23} m^{-3}) the oscillations are absent in the diode without h-BN. In other cases, $\eta_{\max}$ are always higher in the diodes containing a h-BN monolayer.

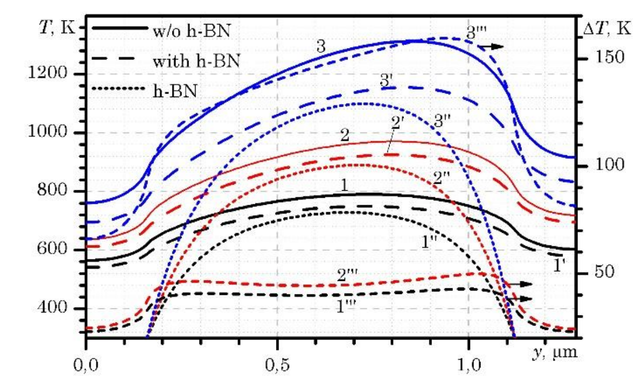

Fig. 4 – Temperature distribution along diode surface at $N_d = 10^{23}$ m^{-3} and different bias (1-3 – diode without SL h-BN; 1'-3' – diode with SL h-BN; 1"-3" – SL h-BN; 1'"-3'" – temperature difference): 1 –$U_0 = 15$ V; 2 – $U_0 = 20$ V; 3 – $U_0 = 22$ V

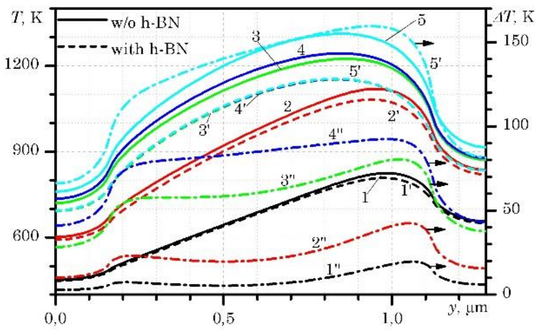

Fig.5. – Temperature distribution along diode surface at U=22 V for different time: (1-5 – without SL h-BN;1'-5' – with SL h-BN; 1''-5'' – temperature difference between cases with and without SL h-BN; 1,1',1'' – t_{sim} = 12.5 ns; 2,2',2'' – t_{sim} = 25 ns; 3,3',3'' – t_{sim} = 50 ns; 4,4',4'' – t_{sim} = 75 ns; 5,5',5'' – t_{sim} = 100 ns

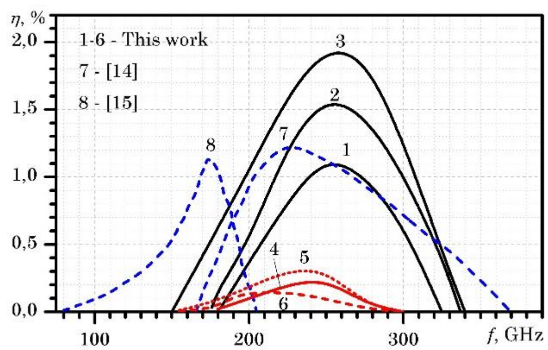

Fig. 6 – Maximal oscillation efficiency vs frequency for different diodes: 1-4, 7-8 – without SL h-BN; 5,6 – with SL h-BN. 1-3,7,8 – without II and heating (1 – $N_d = 6 \times 10^{22}$ m^{-3} (1 μm); 2 – 10^{23} m^{-3} (1 μm); 3 – 2×10^{23} m^{-3} (1 μm); 7 – $N_d = 8 \times 10^{22}$ m^{-3} (0,8 μm); 8 – $N_d = 10^{23}$ m^{-3} (1.2 μm); 4-6 – with II and heating

4. CONCLUSIONS

The results of numerical simulation of the planar GaN n^+-n-n^+ -diode operated in the Gunn-like oscillation mode. The effects of impact ionization and self-heating on efficiency and frequency properties of diodes have been demonstrated. It is concluded that the GaN diode should not be considered without taking those effects into account. In the n^+-n-n^+ diode, the oscillations are suppressed by II at a large bias and high doping. On other hand, self-heating results in the decreasing in mobility and rise of the oscillation voltage threshold. Thus, there is a narrow bias range that can be used for the generation. In most practical cases oscillations are not easy to obtain, that has been demonstrated experimentally [12].

Our simulation shows that using the h-BN monolayer on the top of the diode surface can decrease the local overheating effect. However, it can be only partial solution due to GaN degradation with long-term heating. The high-power operation suggests that the DC IV pulse should be used for obtaining oscillations. The temporary characteristic of such a mode should be considered further. It should be mentioned that the structure of the considered diodes is not optimal for the required temperature distribution and can be enhanced by forming a more uniform electric field in a diode in order to avoid excess heating and permanent device changes.

REFERENCES

1. F. Giannazzo, G. Fisichella, G. Greco, A. La Magna, F. Roccaforte, B. Pecz, R. Yakimova, R. Dagher, A. Michon, Y. Cordier, *Phys. Status Solidi A* **214** No 4, 1600460 (2017).
2. Z. Yan, G. Liu, J.M. Khan, A.A. Balandin, *Nat. Commun.* **3** No 1, 827 (2012).
3. Q. Cai, D. Scullion, W. Gan, et al, *Sci. Adv.* **5** No 6, eaav0129 (2019).
4. J. Tang, J. Zheng, X. Song, L. Cheng, R. Guo, *J. Appl. Phys.* **135** No 20, 205105 (2024).
5. Z. Liu, X. Yu, F. Wang, et al., *Device* **2** No 12, 100520 (2024).
6. M.R. Neupane, D. Ruzmetov, R. Burke, et al, *76th Device Research Conference* (DRC), art. no. 8442141, 1 (Santa Barbara: IEEE; 2018).
7. O. Botsula, K. Prykhodko, V. Zozulia, *IEEE 2nd Ukrainian Microwave Week* (UkrMW 2022), art. no. 10037030, 83 (Kharkiv: IEEE; 2022).
8. A. Park, T. Seo, *Materials* **16** No 22, 7216 (2023).
9. V.O. Zozulia, Y.S. Khodachok, O.V. Botsula, K.H. Prykhodko, *J. Nano- Electron. Phys.* **16** No 6, 06034 (2024).
10. B.F. Donovan, C.J. Szwejkowski, J.C. Duda, et al, *Appl. Phys. Lett.* **105** No 20, 203502 (2014).
11. O.V. Botsula, K.H. Prykhodko, V.A. Zozulia, *Telecomm. Radio Eng+* **76** No 1, 61 (2017)
12. A.S. Hajo, O. Yilmazoglu, A. Dadgar, F. Kuppers, T. Kusserow, *IEEE Access* **8**, 84116 (2020).
13. L. Dobos, B. Pécz, L. Tóth, Zs.J. Horváth, Z.E. Horváth, A. Tóth, E. Horváth, B. Beaumont, Z. Bougrioua, *Applied Surface Science* **253** No 2, 655 (2006).
14. I.P. Storozhenko, Yu.V. Arkusha, *Telecom. Rad. Eng.* **71** No 8, 717 (2012).
15. S. García, I. Íñiguez-de-la-Torre, S. Pérez, J. Mateos, T. González, *J. Appl.* **114** No 7, 074503 (2013).

Генерація у GaN діоді з 2D-h-BN- шаром

В.О. Зозуля, О.В. Боцула, Є.С. Ходачок, К.Г. Приходько, Л.В. Січевська

Харківський національний університет імені В.Н. Каразіна, 61077 Харків, Україна

В роботі ми дослідили роботу гібридного 2D-3D гетероструктурного діода в режимі ганніських коливань. Діод являєє собою структуру на основі GaN, що містить канал n-типову на сапфіровій підкладці з гексагональним моношаром нітриду бору (h-BN), що розташований поверх нього. Моделювання роботи діода було проведено за допомогою багаточастинкового методу Монте-Карло самоузгоджено з числовим розв'язанням системи рівнянь теплопровідності. Використовувалася модель нагрівання на основі макроскопічних теплових параметрів матеріалів. Довжина діода приймалася близькою до 1 мкм, а концентрація донорів – $0,6 \cdot 10^{23}$ – 10^{23} м$^{-3}$. Проведено порівняння характеристик на постійному струмі та коливальних характеристик діодів з моношаром h-BN та без нього. Максимальна ефектив-ність коливань була оцінена в межах можливого діапазону постійних напруг живлення з урахуван-ням ударної іонізації та впливу нагрівання.

Наше моделювання показує, що мікрохвильові коливання в n^{+}-n-n^{+} GaN діоді обмежені ударною іонізацією та саморозігріванням і залежать від напруги живлення та концентрації легуючої домішки. Було отримано розподіли температури в діоді. При вищій концентрації коливання можуть бути повністю придушені ударною іонізацією та ефектом саморозігрівання. Існує вузький діапазон постійних напруг, в якому виникають коливання. Додавання моношару h-BN на поверхню діода може зменшити вплив локального перегріву. Було продемонстровано, що присутність h-BN впливає на величину та перерозподіл температури в прольотній області діода. Діапазон частот, в якому відбувається генерація, звужується, а максимальна ефективність у п'ять разів нижча порівняно з випадком, коли ударна іонізація та самонагрівання не враховується. У деяких випадках за високого легування мікрохвильові коливання з'являються лише в діоді з моношаром h-BN.

Ключові слова: Моношар, GaN, Гетероструктура, Підкладка, Температура, Напруженість електричного поля, Ефект самонагрівання, Ударна іонізація, Коливання, Частотний діапазон.