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InPAs- Based Diode as Active Element in Terahertz Range

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A study of electromagnetic oscillations in the longwave part of the terahertz range by graded-band diodes based on InPAs has been carried out. These diodes contain an InP cathode layer and an InPAs graded-band layer using $InP_{0.2}As_{0.8}$ on the anode contact. Diodes with a length of 500, 640 and 1280 nm were considered. A donor concentration in the active region of the diode is 10^{17} cm^{-3}. The direct current characteristics of diodes were determined and their frequency properties in the oscillation generation mode were evaluated. The simulation was carried out using the Ensemble Monte Carlo Technique with consideration of impact ionization. Characteristics of diodes were compared with those obtained for diodes without accounting for impact ionization.

It was shown that the *I-V* characteristic of short graded-band diodes does not contain areas with negative differential conductivity. Under the condition of impact ionization, these diodes exhibit an increase in current. While these diodes remain stable, they demonstrate charged layer current instabilities and oscillation generation in resonant circuits. The study revealed that the maximum generation efficiency is approximately 10 %, observed in diodes with a length of 1280 nm at a frequency of 100 GHz. In shorter diodes, the efficiency decreases to 3.9 % and 2.0 % in diodes with lengths of 640 and 500 nm, respectively. The cut-off frequency of generation was around 400 GHz in diodes with a length of 500 nm. Impact ionization was found to lead to a decrease in efficiency without compromising the frequency properties of diodes. Conversely, in the case of a 1280 nm diode, it improved frequency properties, supporting the application of graded diodes with impact ionization for achieving maximal frequencies.

Keywords: Graded-gap layer, Electric field strength, Impact ionization, Doping level, Current oscillation, Frequency range, Generation efficiency.

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1. INTRODUCTION

With the increasing prevalence of THz technology, one of the significant tasks is to develop compact radiation sources suitable for integration into compact terahertz systems [1]. Resonant tunnel diodes (RTDs) with a cutoff frequency exceeding 2 THz [2, 3] play a important role in this direction. However, a drawback of RTDs is their relatively low power output. Recently, there has been optimism regarding the usage of quantum cascade lasers (QCLs) [4, 5], which hold promise as sources for various THz applications. However, the main disadvantage of QCLs is their need for additional cooling. The maximum operating temperature for THz QCLs is 250 K in pulse mode [5].

A potential approach is to enhance the characteristics of conventional devices such as Gunn diodes or avalanche transit time diodes (ATTD). Gunn diodes exhibit a significant reduction in alternating current power at a frequency correlated with the inverse intervalley transfer electron times. For instance, employing binary compounds like GaN, InN, and GaN, as well as ternary III-nitride compounds, can yield devices with improved frequency characteristics. However, the experimental realization of gallium nitride-based Gunn diodes remained unresolved for an extended period. The Gunn diode based on GaN of 0.6 μm length has been proposed in [6] where oscillations at the fundamental frequency within the range of 0.3-0.4 THz have been obtained.

In the present day, significant enhancing in device properties can be achieved by utilizing heterostructures, non-lattice-matched materials, and graded semiconductors [7]. The application of graded-band semiconductors in transferred electron devices enhances conditions for electron transport both at the contacts and in the transit region of the diode [8, 9]. Diodes based on graded-band semiconductors can exceed homogeneous diodes in both generation efficiency and frequency properties. Of particular interest are cases involving narrow-gap semiconductors with small energy gap values, such as ternary III-V alloys like GaInAs, AlInN, InPAs, InGaN. Here, InN and InAs exhibit maximal velocities and minimal threshold electric field for electron transfer from the lower valley of the conduction band to the upper satellite ones [10, 11].

Using a narrow-gap semiconductor at the anode contact increases the band gap between nonequivalent valleys. Moreover, these semiconductors have a low threshold energy for impact ionization (II), making impossible fabrication diodes based on InN or InAs for this reason. However, in diodes with graded layers, limited impact ionization may be a factor for improving frequency properties. This phenomenon was demonstrated in a diode with a graded InGaAs layer [12, 13], and also in other device based on homogenous InP [14], and GaAs [15]. In a graded semiconductor of an n-type, the conduction band is flat. Consequently, under applied bias, impact ionization is initiated only by electrons. Furthermore, at moderate applied bias voltages, electrons and holes can move in the same direction toward the anode. At higher applied voltages, some holes move to the cathode, but impact ionization initiated by holes does not occur due to the increasing energy gap and the small force acting on a hole. Consequently, re-

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laxation of electron energy occurs at the anode. The generation frequency was shown to reach up to 320 GHz in a diode with a length of 500 nm [13].

Another possible alternative to GaAs as the fundamental material is to utilize InP and correspondingly replace graded InGaAs with graded InPAs. InP has superior electron velocity in comparison to GaAs and exhibits higher breakdown at the same bias voltage [16].

The objective of this paper is to consider the generation of electromagnetic oscillations in the longwave part of the terahertz region using a graded diode based on the InP/InPAs material system. Additionally, the study aims to investigate the impact of ionization on the output energy and frequency characteristics of these diodes.

2. STRUCTURE AND SIMULATION

Diodes with a length ranging from 0.5 to 1.2 μm have been investigated to determine the maximum oscillation frequencies. Diodes represent structure of n^+- n- n^+- type. According to [13], the concentration in the active n- region was 10^{17} cm^{-3}. The n^+- regions are highly doped areas near the contacts with a donor concentration of $2{\cdot}10^{17}$ cm^{-3}. The importance of the anode concentration has been demonstrated in [13]. Therefore, in the main part of the considered diodes, a concentration of $2{\cdot}10^{17}$ cm^{-3} has been utilized to achieve a high magnitude of force acting on holes in the anode direction.

The coordinate dependence of the alloy composition (mole fraction of arsenic) z in $InP_{1-z}As_z$ is represented as follows:

$$z(x)=\begin{cases}0, & x\le x_0\\ 1-\exp\left(\dfrac{-(x-x_0)^2}{2\sigma^2}\right), & x>x_0\end{cases}, \quad (1)$$

where x_0 – coordinate of heterointerface between homogenous InP and graded InPAs. Estimation of generation efficiency was shown to be maximal for As composition of 0.8 at anode contact. For this reasons, we form composite distribution to obtain value of $z = 0.8$ at the anode by choosing of σ. Distribution (1) looks somewhat similar to heterojunction, especially in case diode of 500 nm length. For this reason, increasing of electron's energy in active region and transfer into satellite valleys is expected to be sufficiently fast.

Diodes modeling is carried out using the Ensemble Monte Carlo Technique (EMC). The primary advantage of this method lies in its ability to account for high-frequency processes in the diode and rapid changes in applied external voltage in the terahertz range. Also, for these purposes, the synchronous ensemble method is employed to determine the free flight time of charge carriers.

Conductivity band is represented three nonparabolicity valleys (Γ, L, X). Dependence of kinetic energy E_K of electron from wave vector module k described by

$$\frac{\hbar^2k^2}{2m^*(z)}=E_K\left(1+\alpha(z)E_K\right), \quad (2)$$

where $m^*(z)$ is an effective electron mass, $\alpha(z)$ is a nonparabolicity factor, and, $\hbar$ – the reduced Planck constant. Here $m^*(z)$ and $\alpha(z)$ are composition functions. Dependences potential energy on composition had been taken in form

$$E_\Gamma(z)=1.35-1.094z-0.1z^2 \quad (3)$$

$$E_L(z)=2.05-0.97z \quad (4)$$

$$E_X(z)=2.21-0.84z \quad (5)$$

Since minimal threshold energy of II E_{th} is determined by heavy holes, it is for this valence zone is presented by heavy holes zone. Zone diagram of the diode of 500 nm length is shown in Fig. 1.

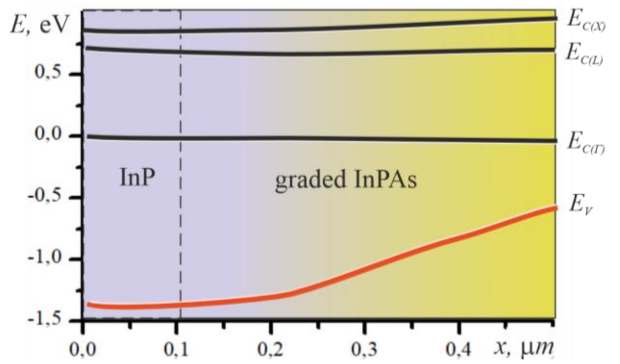

Fig. 1 – Zone diagram of diode with length of 0.5 μm

Capability to use narrows bandgap semiconductor in Gunn diode is known to limit by impact ionization in high field domain. In this case, the current density will be increase with time and after some time Gunn oscillations can become incoherent [17]. In InAs electrons can be heated by an electric field to energies well in excess of the bandgap energy. In contrast, in n- type InAs rate at which holes heat up is limited due to quasi-electric field and the relatively flat heavy hole band. It is evidence from the Fig. 1, the usage one zone to describe valence zone is possible if bias voltage will be applied to diode.

Threshold energy of II in InPAs is depended on crystallographic orientation and limited by the nonparabolicity factor [18].

$$E_{th}(z)=\frac{(1+\gamma)}{2\alpha(z)}\left[1\pm\sqrt{1-4\alpha(z)E_g(z)(2+\gamma)/(1+\gamma)^2}.\right], (6)$$

where $\gamma=\gamma(z)$ is electron effective mass to hole effective mass ratio. The probability of ionization $W_{II}(E)$ is defined approximately in the manner

$$W_{II}(E,z)=W_0(z)(E-E_{th}(z))^n, \quad (7)$$

where $W_0(z)$ and n are material dependent, and known as the fitting or softness parameters. The Keldysh approach ($n=2$) is used, which demands a hard threshold for II. In the present report, initial stage of II is considered, and the assumption is applicable. Cristal orientation (direction from cathode to anode) is suggested to be [1 1 1], as a result, II was considered in Γ-valley and X- valleys only.

The most importance scattering mechanisms as scattering on deformation potential of nonpolar optical phonon and acoustic phonon, polar optical phonon scattering, intervalley scattering, alloy disorder and ionized impurity scatterings were accounted. The material parameters used in numerical model correspond to [12].

A 2D model was employed for diode simulation. The improved cloud-in-cell (CIC) scheme for charge assignment was implemented to enhance spatial accuracy in the presence of spatially dependent permittivity, along with self-force reduction. To found 2D-potential distribution $\varphi(x,y)$, the full multigrid (FMG) method for solving of Poisson equation providing results as fast as possible was used [19].

3. RESULT AND DISCUDION

Dependence of the current density on the applied bias for InP/InPAs- based diodes without II and with II, for different diode lengths 500 nm, 640 nm and 1280 nm, are shown in Fig. 2.

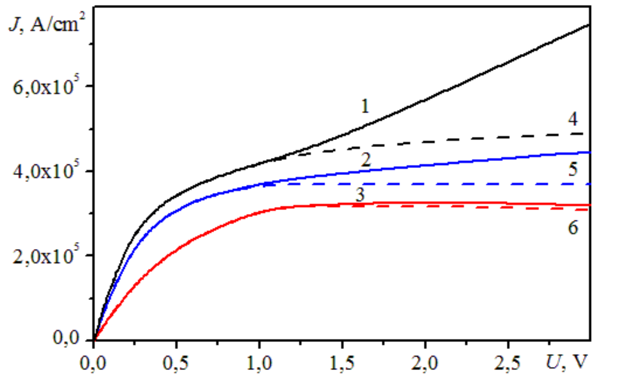

Fig. 2 – Current density J versus bias voltage U for diodes with difference length, with II – 1-3, without II – 4-6; 1, 4 – 500 nm, 2, 5 – 640 nm, 3, 6 – 1280 nm

From the observed increase in current density, it can be concluded that the II is dominant factor to form *I-V* – characteristic. In considered diode, impact ionization is initiated only one carrier type. It is characteristically different from case when both carrier types can cause impact ionization. This results in an exponentially rising current without an avalanche breakdown.

The energy diagram of InP/InPAs heterostructure diode, energy distribution of change carriers and number of impact ionization events (in arbitrary units) at bias voltage of 1 V, is shown in Fig.3.

Dependence $E_C(z)$ and $E_V(z)$ determine main components of quasi- electric fields in conduction band and valence band correspondently. As seen in Fig. 3, ionization occurred near anode contact. In this region, the quasi-electric field in the valence band acts in the opposite direction compared to other parts of the diode. Electrons and holes are pulled in the same direction, toward the anode. Minority of hole moves to cathode, but cannot obtain enough kinetic energy to carry out the act of impact ionization. Thus, the hole current is the algebraic sum of the current associated with holes moving into the anode and the current due to holes that were transited toward the cathode.

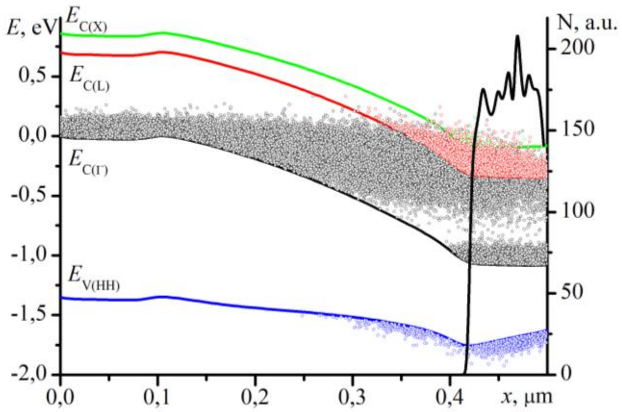

Fig. 3 – Energy diagram of diode, distributions carriers in valleys, and number of impact ionization acts in diode with 500 nm length at bias voltage of 1 V

Since the impact ionization process is influenced by the energy of a carrier, the probability of impact ionization decreases as the diode length increases. This is due to both the increased fre-quency of phonon scattering and the smaller force acting on electrons. As a result, the current rise due to impact ionization is not observed in a diode of 1280 nm. Moreover, in this case, a small current drop occurs at a large bias voltage. In shorter diodes, the DC differential resistance is positive, and the current rises as the diode length decreases. The linear rise of current on this scale is caused by the dominance of impact ionization of just one carrier type (electrons). In fact, the multiplication factor M_n for electrons cannot exceed 2, and the probability of a hole making even one act of impact ionization is practically zero. Thus, II can be considered as a way of energy relaxation.

Energy and frequency characteristics of diodes can be estimated by considering their operation in the oscillation mode. In this mode, the diode structure is assumed to be placed in a resonator, and the applied voltage $U(t)$ acting on the structure is the sum of the constant bias voltage U_0 and the alternative voltage $U(t)$. Resonator is suggested to have high quality factor Q, therefor, $U(t)$ represents the first harmonic with frequency f and amplitude U_1:

$$U(t) = U_0 + U_1 \sin 2\pi f t \qquad (8)$$

Due to relatively strong current grooving at high bias voltage, the voltage range corresponding continue mode can be bounded from above. It mainly takes place for short diode which are always stable at $U_1 = 0$. Current instabilities are raised at bias that is greater than some critical value U_p. U_p is estimated in excess of 1.25 V for diode of 500 nm, and in excess of the 1.3 V for diode of 500 nm, and it depending on the frequency.

Electric field distribution along the diode of 500 nm at difference time moments during an oscillation period is shown in Fig. 4.

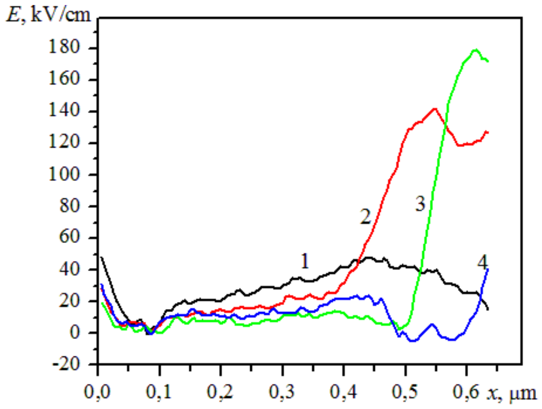

Fig. 4 – Electric field distribution in diode of 640 nm, $U_0 = 2.25$ V, $U_1 = 1$ V: 1 – $t = 0$; 2 – $t = T/4$; 3 – $t = T/2$; 4 – $t = 3T/4$

The distributions were obtained at optimal values of voltage and resonator frequency. The primary type of current instabilities in diodes is the formation of accumulation layers. Accumulation layers form mainly in the second half of graded layer, where the electric field strength is higher, particularly in the anode region of 200 nm. This width corresponds to the region where impact ionization (II) is the dominant process.

However, in diode of 1280 nm self-oscillations of current are also observed at voltage upper then 2.6 V. This fact can be associated with static negative resistance in those diodes. Frequency of oscillation is about 150 GHz. At less bias voltage oscillations are damped. In resonance regime, for diode of 1280 nm, U_p exceeds 1.3 V.

The high frequency properties of the diode were evaluated by determining the oscillation efficiency (η) at the corresponding resonator frequency. η was calculated as a ratio of the power generated at the resonator frequency (first harmonic) to the average direct current power. To find the maximum efficiency, optimization was carried out by variation of bias U_0 and amplitude U_1. To estimate of effect of impact ionization on diode generation, the characteristic without impact ionization are received too. Dependencies of the optimized oscillation efficiency on resonator frequency are shown in Fig. 5, and Fig. 6. Donor concentration in all diodes is the same, and equaled 10^{17} cm^{-3}.

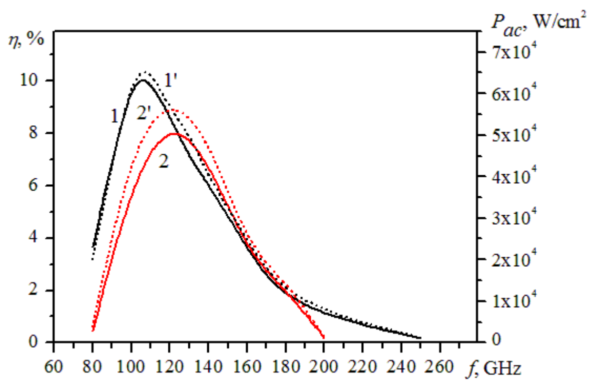

Fig. 5 – Frequency dependence of maximal oscillation efficiency (1, 2) and ac power density (1', 2') in diode of 1280 nm: 1, 1' – with II, 2, 2' – without II

As can be seen from the figure, peak efficiency η_{max} for long diode can reach 10 %, and is corresponded to $f_0 = 100$ GHz. Oscillation is observed in a range from 70 to 250 GHz. The optimal bias voltage for all considered diodes is (2...3) U_p that corresponded to Gunn effect in homogeneous diode.

Oscillation frequency is increase as diode length decreases, $f_0 = 180$ GHz for diode of 640 nm, and $f_0 = 250$ GHz for diode of 500 nm. Maximum of efficiency are 3 %, and 1.3 % correspondently. Diodes have a wide frequency range. Thus, it is from 120 to 350 GHz for diode of 640 GHz, and, from 140 to 400 GHz for diode of 500 nm. The highest value of cutoff frequency amount considered length can be obtained for diode of 500 nm, and is 400 GHz. This value is higher than in graded InGaAs- based diodes with the same parameters considered in [13] for which cutoff frequency was 350 GHz.

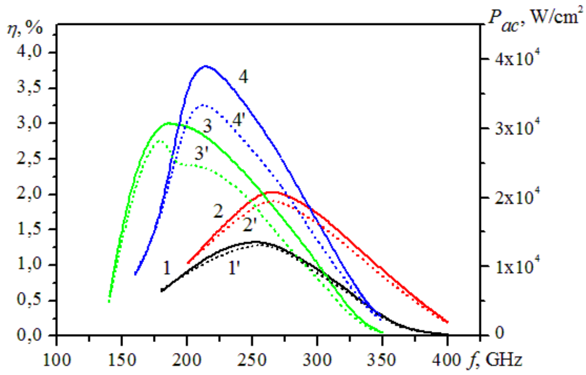

Fig. 6 – Frequency dependence of maximal oscillation efficiency (1-4) and ac power density (1'-4') in diode of 500 nm (1, 1', 2, 2'), and 640 nm (3, 3', 4, 4') accordantly: 1, 1', 3, 3' – with II, 2, 2', 4, 4' – without II

II is expected to influence on upper-frequency limit of oscillation frequency. In fact, increasing of cutoff frequency, when compared to diodes without II, is observed only in long diodes. Consequently, cutoff frequency was achieved up to 250 GHz (200 GHz in the case of simulation diodes without II). In short diodes, the cutoff frequency remains the same, but the magnitude of efficiency is lower than in the simulation of diodes without II.

As can be seen from simulation results, shown in Fig.5 and Fig. 6, oscillation efficiency in diodes with II is shifted to lower values in all considered cases. At the same time, the bias voltage corresponding to maximal efficiency in diode with II is lower than in case of the diode without II.

4. CONCLUSIONS

We present the result of Monte Carlo simulation of graded-gap InPAs diodes. Our investigation demonstrates that graded-gap diodes, with InP on the cathode and the narrow-gap semiconductor $InP_{0.2}As_{0.8}$ at the anode contact, can be used as an effective active elements for oscillation generation in the lower part of the terahertz range. The transfer electron effect is considered to be a reason for the appearance of oscillations. The cutoff frequency of generation reaches 400 GHz when a diode with a length of 500 nm is used. The diodes exhibit a wide frequency range of over 100 GHz.

The impact ionization effect on the possibility of obtaining generation was also considered. In some cases, this process can enhance the frequency properties of the diode, as observed in graded InGaAs-based diodes [13]. In our consideration, a simple model of impact ionization is used, which accounts for the relaxation process only in the lower Γ-valley and satellite X-valley. However, there is a dramatic anisotropy of impact ionization. Therefore, impact ionization in the L-valley may also play an important role in the energy relaxation of hot electrons. This aspect needs to be analyzed in future studies, as it could lead to changes in our estimations. The second important factor influencing the results could be the self-heating effect arising due to the strong field in the anode region. It is suggested that this effect may play a significant role in long diodes and should be considered in simulations as well.

REFERENCES

1. L.F. Shi, A. Zahid, A. Ren, et al., *Phys. Scripta* **98**, No 6 065006 (2023).
2. M. Asada, S Suzuki, *Sensors* **21** No 4, 1384 (2021).
3. R. Izumi, S. Suzuki, M Asada, *42nd International Conference on Infrared, Millimeter, and Terahertz Waves (IRMMW-THz 2017)*, art. no. 17259158, 1 (Cancun: IEEE: 2017).
4. M.S. Vitiello, A. Tredicucci, *Adv. Phys.: X* **6** No 1, 1893809 (2021).
5. A. Khalatpour, A.K. Paulsen, C. Deimert, et al., *Nat. Photon.* **15**, 16 (2021).
6. A.S. Hajo, O. Yilmazoglu, A. Dadgar, et al., *IEEE Access* **8**, 84116 (2020).
7. F. Capasso, *Electronic Structure of Semiconductor Heterojunctions. Perspectives in Condensed Matter Physics 1* (Dordrecht: Springer Netherlands: 1988).
8. I. Storozhenko, *J. Nano- Electron. Phys.* **12**, No 1 01015 (2020).
9. K.H. Prykhodko, V.O. Zozulia, O.V. Botsula, *International Young Scientists Forum on Applied Physics and Engineering (YSF–2017)*, art. no. 17413958, 291 (Lviv: IEEE: 2017).
10. O.V. Botsula, K.H. Prykhodko, *2020 IEEE Ukrainian Microwave Week (UkrMW 2020)*, art. no. 9252763, 925 (Kharkiv: IEEE; 2020).
11. I. Storozhenko, S. Sanin, *J. Nano- Electron. Phys.* **14** No 1 01027 (2022)
12. O.V. Botsula, K.H. Prykhodko, V.A. Zozulia, *J. Nano-Electron. Phys.* **11** No 1, 01006 (2019).
13. O. Botsula, K. Prykhodko, V. Zozulia, *3rd Ukraine Conference on Electrical and Computer Engineering (UKRCON 2021),* art. no. 21388452, 504 (Lviv: IEEE; 2021).
14. S. Asmontas, V. Gružinskis, P. Shiktorov, et al, *The 31st International Conference on the Physics of Semiconductors (ICPS 2012)*, 385 (Zurich: AIP Publishing LLC: 2012).
15. V. Gružinskis, E. Starikov, P. Shiktorov, *Lith. J. Phys.* **54** No 1, 7 (2014).
16. I. Vurgaftman, J.R. Meyer, L.R. Ram-Mohan, *J. Appl. Phys.* **89** No 11, 5815 (2001).
17. M. Levinshtein, J. Kostamovaara, S. Vainshtein, *Breakdown Phenomena in Semiconductors and Semiconductor Devices* (Singapore: World Scientific: 2005).
18. K. Brennan, N. Mansour, *J. Appl. Phys.* **69** No 11 7844 (1991).
19. W. Joppich, S. Mijalković, *Multigrid Methods for Process Simulation* (Vienna: Springer: 1993).

Діод на основі InPAs як активний елемент терагерцового діапазону

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Проведено дослідження електромагнітних коливань у довгохвильовій частині терагерцового діапазону варізонними діодами на основі InPAs. Ці діоди містять InP катодний шар шар та варізонний шар InPAs з використанням $InP_{0.2}As_{0.8}$ на анодному контакті. Розглядалися діоди довжиною 500, 640 і 1280 нм. Концентрація донорів в активній області діода становить 10^{17} см$^{-3}$. Визначено характеристики діодів на постійному струмі та оцінено їх частотні властивості в режимі генерації коливань. Моделювання проводилося за допомогою багаточасткового методу Монте – Карло з урахуванням ударної іонізації. Характеристики діодів порівнювались з отриманими для діодів без урахування ударної іонізації.

Показано, що ВАХ коротких варизонних діодів не містить області з негативною диференціальною провідністю. В умовах ударної іонізації ці діоди демонструють збільшення струму. Хоча ці діоди залишаються стабільними, у резонансних контурах вони демонструють нестійкості струму типу зарядженого шару та генерацію коливань. Дослідження показало, що максимальна ефективність генерації становить приблизно 10 %, спостерігається в діодах довжиною 1280 нм на частоті 100 ГГц. У більш коротких діодах ефективність знижується до 3,9 % і 2,0 % у діодах довжиною 640 і 500 нм відповідно. Гранична частота генерації була близько 400 ГГц в діодах довжиною 500 нм. Було виявлено, що ударна іонізація призводить до зниження ефективності без погіршення частотних властивостей діодів. І навпаки, у випадку діода 1280 нм вона покращує частотні властивості, дозволяючи застосування варізонних діодів з ударною іонізацією для отримання максимальних частот.

Ключові слова: Варізонний шар, Напруженість електричного поля, Ударна іонізація, Рівень легування, Коливання струму, Частотний діапазон, Ефективність генерації.