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Generation of Electromagnetic Oscillations of Submillimeter Range by $Ga_zIn_{1-z}As$ Diodes Using Impact Ionization

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Development of millimeter and terahertz wave ranges is one of the main objectives of modern high-frequency electronic devices. However, there are not many active elements able to operate in these ranges. Transferred electron devices (TED) still remain a more widespread compact electromagnetic wave sources. But oscillation efficiency of TED operating in the submillimeter wave range is small and, in most cases, generation becomes impossible.

Difficulties in obtaining maximum frequencies are mainly determined by the electron transition time from the upper valley to the lower one. The aim of the work is to investigate reduction of the transition time problem by using band to band impact ionization. The paper deals with charge transport in short diodes with $In_zGa_{1-z}As$-based graded band structure with the active region length of 0.64 μm. Doping concentration in the *n*-type active region was $10^{16}…8\cdot10^{16}$ cm^{-3}. Ensemble Monte-Carlo Technique is carried out to describe the charge carrier dynamics in the device. A three-valley conduction band and heavy hole band Γ_{V1} are taken into account.

It is shown a possibility of using localized impact ionization as an energy relaxation mechanism. Correlation between the number of acts of impact ionization and decrease in electron number in the upper valleys are demonstrated. Oscillation efficiency of the diodes is calculated. It is shown that impact ionization can lead to increase in the maximum generation frequency.

The proposed way of improving frequency properties due to modification of electron transfer near the anode contact can be applied to short structures and allows maximum generation frequencies.

Keywords: Diodes, Impact ionization, Graded-gap layer, Domain, Electric field strength, Generation efficiency, Frequency range.

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1. INTRODUCTIION

Diodes based on electron transfer to the upper valleys (TED or Gunn diodes) are most common sources of microwave oscillation in centimeter and millimeter bands.

Spectral characteristics of TED are the best among solid-state devices used for generating in these ranges. The most usable materials for manufacturing diodes are gallium arsenide (GaAs), indium phosphide (InP) and other semiconductors possessing the appropriate features of the band structure. Conduction zone consists of several valleys. Effective mass of the upper valley is greater than that of the lower Γ-valley. Another requirement is an energy gap between the valleys ΔE which is quite big. Transition of electrons into a valley with a greater effective mass leads to decrease in mobility of electrons and their velocity in a certain part of the diode. This leads to a periodic formation of high-ohmic domain and occurrence of current fluctuations [1]. Oscillation frequency in most cases is determined by existence time of a high-ohmic nonhomogeneity. If nonhomogeneity passes through a diode, oscillation period also depends on the diode length.

Efficiency of TED operating in the submillimeter wave range is small and in most cases, generation becomes impossible.

There are several reasons to reduce efficiency [2, 3]. The first one is that when the electric field intensity increases, electrons do not have time to gain quickly the needed energy for intervalley transition. Therefore, when the field is low, electrons cannot quickly move from the upper valley to the lower one. The second reason is the existence of a "dead zone". This is a distance that an electron passes in an electric field to obtain energy ΔE corresponding to the energy gap between the central and lateral valleys.

Resistance of the diode "dead zone" region is positive; it is connected consequently with negative resistance of the diode active part in generation mode. This problem is usually solved by changing a crystal structure on the cathode contact and creating a strong field region near the cathode [4]. One more way is an increase in electron energy due to passing through the boundary of two semiconductors with different band gaps (heterojunction) [5, 6].

Difficulties in obtaining maximum frequencies are entirely determined by the first reason. [1] Transition times are known to decrease from the central to the lateral valley with increasing electric field. Accordingly, they can be reduced in the same way due to the length of the "dead zone". Particularly, to reduce direct transition time, semiconductor layers with variable composition can be used, so that the energy gap between the lower and lateral valleys is minimal at the cathode and increases in the direction of the anode. Examples of graded gap $Al_zGa_{1-z}As$, GaP_zAs_{1-z} and $In_zGa_{1-z}As$-based diode usage are presented in works [7-9].

The problem of the above structures is that transition time from the upper valley to the lower one is determined by material at the anode contact. Therefore, transition time from the upper valley to the lower one is the same as in the diode entirely made of homogeneous material.

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The purpose of this work is to investigate reduction of the transition time problem by using band to band impact ionization.

2. DIODES STRUCTURE AND THEIR NUMERICAL MODEL

In the case of TED, impact ionization, which arises in the area of spatial charge wave formation, usually leads to disappearance of current fluctuations. The main negative factor is increasing concentration of charge carriers, both electrons and holes, and their accumulation in the active diode region. This leads to an increase in positive conductivity.

In short diodes, this negative effect can be avoided due to localization of impact ionization near the anode. It is known that final distribution of electrons between valleys is determined by density of states. It is much smaller in the Γ-valley than in the X-L ones due to a small effective mass of electrons. In the upper lateral X-L valleys, relaxation rate of energy is large due to a significant intensity of inter-valley and intro-valley scatterings. Therefore, electrons in the equilibrium state will be located mainly in minima of the lateral X-L-valleys. In this case, the electron initiated impact ionization in the anode region can lead to their energy relaxation and transition intensity decreases in the lateral valleys. The electron initiated impact ionization in the X-valley results in a decrease in their number in the X-valley and their transition to the Γ-valley (electron initiated impact ionization in the L-valley is not possible due to specificity of the band structure). In the end, taking into account electron exchange between the X and L valleys, the impact ionization can lead to a fast transition of electrons from the upper valleys to the lower ones.

To implement this mechanism, two conditions should be realized: 1) the impact ionization has to occur in the anode contact region; 2) the charge carriers resulting from the impact ionization have to leave the diode within a time interval of less than half of the oscillation period.

To satisfy the first condition, it is necessary that the diode's material composition varies to reduce the band width to the desired value for impact ionization occurrence at the anode contact. The second condition is fulfilled also as a quasi-electric field of graded semiconductors acting predominantly on holes in the n-type semiconductor layer. As a result, both electrons and holes move towards the anode contact [10]. This limits propagation of the positively charged charge carriers (holes) into the diode.

The best conditions in this case correspond to a situation when half of the oscillation period is close to the electron energy relaxation time and the hole drift time to the anode contact.

$Ga_zIn_{1-z}As$-based diode structures proposed in [11] are taken into account. The diode doping profile a) and distribution of gallium fraction z in $Ga_zIn_{1-z}As$ b) are shown in Fig. 1.

The doping concentration in the n-type active region is $10^{16}...8\cdot10^{16}$ cm^{-3}, the concentration in the n^+-cathode and the n^+-anode is 10^{17}-10^{18} cm^{-3}, respectively. The total diode thickness is 1.28 μm, while the active region length is 0.64 μm.

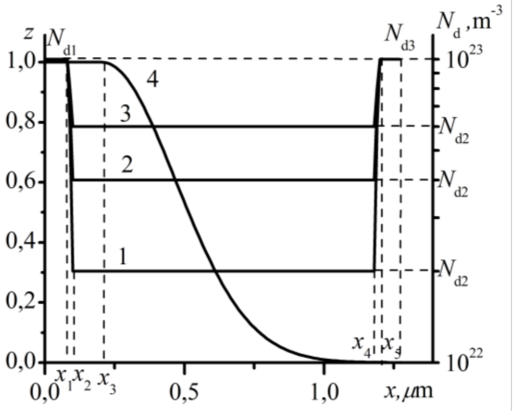

Fig. 1 – Distributions of doping profiles and Ga fraction: 1-3 – considered doping profiles, 4 – Ga fraction versus coordinate

Ensemble Monte-Carlo Technique (EMC) is carried out to describe the charge carrier dynamics in the device and determine energy and frequency characteristics of the diode modeling. All transport equations, material parameters and model peculiarities corresponded to [11, 12]. A three-valley conduction band, the lower (Γ) and upper X and L-valleys are taken into account. For all the considered valleys, a zone nonparabolicity is given in a form:

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

where k is the electron wave vector module, α is a nonparabolicity factor, m^* is the effective electron mass, $\hbar$ is the reduced Planck constant. Band-structure-related parameters used in the simulation, such as the energies at the symmetry points Γ, L, X, the effective density of state masses in units of the free electron mass m_0 and the nonparabolicity parameter, are presented in Table 1.

Table 1 – Band structure parameters

Parameter	Valley	Value
Valley minimum, eV	Γ	$0.356 + 0.581z + 0.502z^2$
	L	$1.08 - 0.129z + 0.818z^2$
	X	$1.37 - 0.684z + 1.275z^2$
Non-parabolicity factor, eV^{-1}	Γ	$(1 - m_\Gamma^*)^2/\varepsilon_\Gamma$
	L	$0.65z + 0.54(z - 1)$
	X	$0.36z + 0.9(z - 1)$
Effective mass, m^*/m_e	Γ	$0.023 + 0.037z + 0.003z^2$
	L m_l (m_t)	$1.32 + 0.58z(0.28 - 0.2046z)$
	X m_l (m_t)	$3.57 - 2.27z$ $(0.12 + 0.11z)$
	Γ_{V1}	$0.548 + 0.034z$

The main difference from [11] is the usage of the valence band represented by parabolic heavy hole zone Γ_{V1}.

It is assumed that parameters of the $Ga_zIn_{1-z}As$ semi-conductor compound vary with position in accordance to the $z(x)$ law. However, parameters remain constant within the spatial cell and are equal to the value in the middle of the cell when scattering process happens.

Deformation potential (acoustic and optic), polar optical phonon, intervalley, alloy disorder and ionized impurity scattering were taken into account. The main scattering parameters used in the simulation are listed in Table 2.

Table 2 – Scattering parameters

Parameter	Valley	Value
Acoustic wave velocity, m/s		$4280 + 960z$
Acoustic deformation potential, eV	Γ	$7z + 5.8(1 - z)$
	L	$9.2z + 5.8(1 - z)$
	X	$9.27z + 5.8(1 - z)$
Optical deformation potential, eV/m	Γ	0
	L	$(0.3z + 1(1 - z))10^{11}$
	X	0
Optical phonon energy, eV		$0.0343z + 0.03128(1 - z)$
Intervalley coupling constant, m^*eV^{-1}	Γ–L	$(0.65z + 1(1 - z))10^{11}$
	Γ–X, L–L	10^{11}
	L–X	$(0.5z + 0.9(z - 1))10^{11}$
	X–X	$(0.7z + 0.9(z - 1))10^{11}$
Intervalley phonon energy, eV	Γ–L	0.0278
	Γ–X	0.0299
	L–L	0.029
	L–X	$0.0278z + 0.0293(1 - z)$
	X–X	0.0299

Impact ionization accounts both Γ and X-valleys. But, it is limited by the nonparabolicity factor in X-valleys [13]. According to the proposed Ga distribution in $Ga_zIn_{1-z}As$, impact ionization becomes possible only in the anode contact region that enables us to obtain a rapid inter-valley relaxation in this part of the diode. The Ga fraction in the $Ga_zIn_{1-z}As$ in the $x_3 - x_5$-region is normally distributed (see Fig 1, curve 4). These conditions are similar to a heterojunction near the cathode and lead to increase in the electron energy and its transition to the upper valleys. A more important thing is that this distribution forms a graded layer on the anode creating a quasi-electric field in the n active region and n^+ anode acting on a hole in the anode direction. Thus, rapid removal of holes from the diode takes place and it prevents their accumulation in the diode.

3. GENERATION EFFICIENCY OF DIODES

To investigate operation of the diode in the oscillation modes, the diode resonator is considered. The effect of the resonator is taken into account by applying to the diode of the corresponding voltage in the form

$$U(t) = U_0 + U_1 \sin \omega t , \qquad (2)$$

where U_0 is the bias voltage, U_1 is the alternative voltage amplitude (first voltage harmonic) determined by the resonator, f is the resonator frequency. Oscillation efficiency is determined as

$$\eta = \frac{P_{\square}}{P_0} \cdot 100\% , \qquad (3)$$

where $P_{\square}$ is the power generated by the diode at the resonator frequency, P_0 is the direct current power. Maximum generation efficiency is stated by optimizing the values of bias voltage and the first harmonic amplitude.

Distributions of the relative number of impact ionization acts in the diode and distributions of the relative electron concentration in L-valleys are shown in Fig. 2.

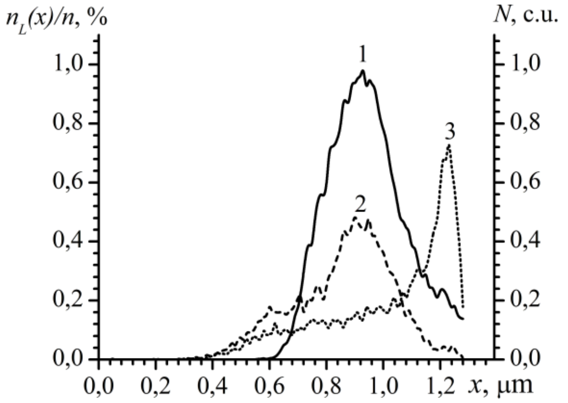

Fig. 2 – Distributions of relative number of impact ionization acts in the diode – 1, relative electron number in satellite valley – 2, 3: 2 – without impact ionization; 3 – with impact ionization at $U_0 = 1.5$ V , $U_1 = 0.6$ V

Dependence of the relative electron concentration in L-valleys on coordinate is given also for the case without impact ionization. As it can be seen, increase in the number of impact ionization acts completely correlates with decrease in the electron number in the upper L-valleys. All these results support the argument that impact ionization can strongly effect the relaxation processes in the diode. Moreover, this influence occurs both directly (relaxation in the X-valleys) and indirectly (relaxation in the L-valleys) due to high intensity of inter-valley scattering.

Frequency dependence of the oscillation efficiency on resonator frequency at fixed diode voltages is given in Fig. 3 with and without consideration of impact ionization process.

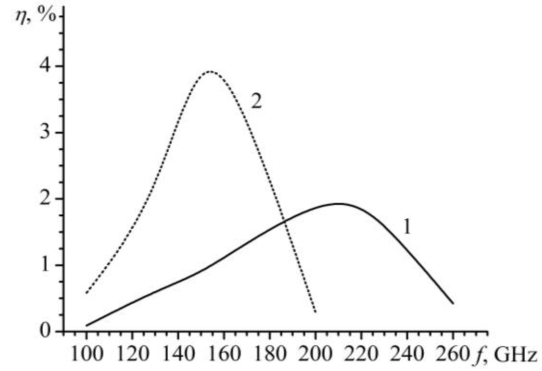

Fig. 3 – Frequency dependence of diode generation efficiency at bias voltage $U_0 = 1.5$ V and $U_1 = 0.4$ V, 1 – with impact ionization; 2 – without impact ionization

It seems that Ga_zIn_{1-z}zAs-based graded band diode by itself is a very high-frequency device. This fact is associated mainly with its good velocity-field characteristic. Theoretical studies of $Ga_zIn_{1-z}As$-based TEDs indicate that frequency limits of such devices can be greater than for GaAs (150 – 155 GHz in the LSE mode). Theoretically, it is expected that impact ionization limits transfer electron effect at $x < 0.3…0.4$ [14], but these estimations have been done for a fairly long diode structure and the non-local effects that take place into short diodes have not been taken into account [14]. In the considered diode, impact ionization near the anode contact leads to expansion of the frequency range of the diode. Maximum frequency shifts towards higher ones.

Frequency dependences of oscillation efficiency for the diode with different doping levels of the active region are shown in Fig. 4.

There is optimum concentration for both maximum efficiency and frequency range. Maximum efficiency is above 5 % and corresponds to the doping concentration in the active region $Nd_2 = 4\cdot10^{15}$cm^{-3}. Increase in electron concentration leads to increase in maximum frequency value but it is accompanied by efficiency degree.

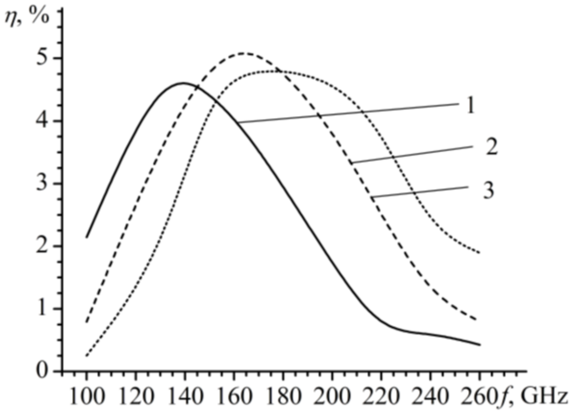

Fig. 4 – Dependence of generation efficiency on frequency for the diodes with different doping levels of the *n*-region: 1 – $Nd_2 = 2\cdot10^{15}$ cm^{-3}; 2 – $Nd_2 = 4\cdot10^{15}$ cm^{-3}; 3 – $Nd_2 = 6\cdot10^{15}$ cm^{-3}

4. CONCLUSIONS

Traditional generation device like TEDs still remains a more solid electromagnetic wave source. To obtain higher frequency characteristics, TED's structure is constantly improved. The proposed way of improving frequency properties due to modification of electron transfer near the anode contact can be applied to short structures and allows maximum generation frequencies. Moreover, in the case of short structures, the process involving holes can be neglected. Possible limits are determined by the existence of a distance, which is frequently referred to a "dead length" [15]. A carrier needs to travel this distance to gain sufficient energy for impact ionization act. The ionization region size cannot be smaller than a dead length. Also, there is a limit connected to growth difficulties of small width of Ga$_z$In$_{1-z}$As-based structures. Ga$_z$In$_{1-z}$As layers are not the lattice matched to GaAs. Therefore, the layer with graded composition is necessary to achieve epitaxial growth on GaAs substrates at low In concentrations. At high In concentrations (more than 53 %), an InP buffer layer is necessary.

As for cathode contacts applied jointly with the proposed method, usage of high ohmic regions looks like a narrow region near the cathode, where the doping level is lower than the active region that is undesirable due to strong influence of impact ionization in the short diode. Heterostructure contacts are preferred over the other ones. Possible variants are graded structures [8] or a complex structure like the resonance tunneling diode [16].

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Генерація електромагнітних коливань субміліметрового діапазону діодами Ga$_z$In$_{1-z}$As з використанням ударної іонізації

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Розвиток міліметрового і терагерцового діапазонів хвиль є одним з головних завдань сучасних високочастотних електронних приладів. Проте, немає активних елементів, які можуть працювати в цих діапазонах. Пристрої з переносом електронів (ППЕ) все ще залишаються більш поширеними компактними джерелами електромагнітних хвиль. Але ефективність коливань ППЕ, що працюють у субміліметровому діапазоні хвиль, невелика, і в більшості випадків генерація стає неможливою.

Труднощі отримання максимальних частот в основному визначаються часом переходу електрона від верхньої долини до нижньої. Метою роботи є дослідження зменшення часу переходу електрона шляхом використання міжзонної ударної іонізації. У роботі розглянуто перенесення заряду в діодах зі змінною шириною забороненої зони на основі $In_zGa_{1-z}As$ з довжиною активної області 0.64 мкм. Концентрація домішки в активній області n-типу становила 10^{16}-$8\cdot10^{16}$ см$^{-3}$. Метод Монте Карло для моделювання поведінки ансамблю частинок застосовується для опису динаміки носіїв заряду в пристрої. При цьому враховуються триполосні зони провідності і смуги важких отворів Γ_{V1}.

Показано можливість використання локалізованої ударної іонізації як механізму енергетичної релаксації. Продемонстровано взаємозв'язок між кількістю актів ударної іонізації та зменшенням кількості електронів у верхніх долинах. Розраховано ефективність коливань діодів. Показано, що ударна іонізація може призвести до збільшення максимальної частоти генерації.

Запропонований спосіб удосконалення частотних властивостей за рахунок модифікації транспорту електронів поблизу анодного контакту може бути застосований до коротких структур і дає можливість отримати максимальні частоти генерації.

Ключові слова: Діоди, Ударна іонізація, Шар зі змінною шириною забороненої зони, Домен, Напруженість електричного поля, Ефективність генерації, Діапазон частот.