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Graded-gap AlInN Gunn diodes

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> **Abstract.** The paper deals with the numerical simulation of Gunn diodes operation based on the graded-gap AlInN. We have obtained the output characteristics of diodes with different cathode contacts in a wide range of frequencies. Harmonic and biharmonic modes of operation have been considered. Cutoff frequency and minimum length of the active region have been estimated. Performances of graded-gap AlInN diodes are compared with the performances of InN and AlN diodes.

> **Keywords:** Gunn diode, transfer electron device, graded-gap semiconductor, nitride semiconductor, intervalley electron transfer, terahertz range.

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1. Introduction

Nitrides of group III elements attract attention as promising materials for various high-speed electronic devices, including devices based on the intervalley electron transfer (IET) effect. These materials include AlN, InN and GaN. Transport properties of these compounds have been extensively studied by numerical simulation methods, e.g. in papers [1-4]. Good inertial properties and high drift velocities of charge carriers are mentioned in all publications. In a number of studies [5-9], numerical experiments on the microwave generation using Gunn diodes (TED, transfer electron device) based on semiconductor nitrides have been carried out. The above studies show prospects of such devices for a terahertz range. At the same time, there are very few experimental studies of semiconductor nitrides higher than the threshold values of the electric field. We can name only few studies [10, 11], where the current-voltage characteristic has been observed above the threshold field in the pulsed mode, and the measurements of negative differential conductivity in GaN have been carried out. As far as we know, there are no researches on experimental microwave generation based on the IET effect. The primary problem that does not allow obtaining the microwave generation is to remove heat from the active region of the device [8, 9]. Another important unresolved problem is the heating the electron gas at the cathode contact. The means proved to be successful with TED based on GaAs or InP turned out to be inefficient for semiconductor nitrides [8]. One of the weakly-studied directions in the area of TED creation is the use of gradedgap semiconductor compounds that can overcome the need of heating to some extent for the electron gas at the cathode [12-15]. So, there is a need to study the microwave generation of TED based on graded-gap semiconductor nitrides, in particular, AlInN, by numerical simulations aimed at determining prospects and possibilities of practical realization of these devices.

2. Setting the problem and parameters

The choice of AlInN compound is caused by the following reasons. Among semiconductor nitrides with a hexagonal crystal lattice (wurtzite modification), InN possesses the maximum drift velocity of electrons and the minimum threshold value of the electric field [1-3, 8]. InN concedes to GaN and AlN as to inertial properties of IET and the probability of IET overlap by impact ionization. According to estimations [6, 8], TED based on InN should be of a better performance in the near-terahertz range.

To prevent IET overlap by impact ionization, it is expedient to use the ternary compounds InGaN or InAlN, which increases the band gap but reduces the electron mobility. To improve the generation efficiency, it is preferable to use graded-gap compounds with widening the coordinate energy gap between nonequivalent valleys. AlN compound has a narrower energy gap between the central valley and the nearest by its energy to it side one by 0.6 eV than that of GaN. This has determined the choice of AlN as a pair to InN.

The percentage of InN in $Al_{1-x(z)}In_{x(z)}N$ compound is defined by dependence

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$$x(z) = (x_1 - x_2) \left[1 + \exp\left(\frac{4(z - z_0)}{l_v}\right) \right]^{-1} + x_2,$$
(1)

where x_1 and x_2 are boundary contents of InN at $-\infty$ and $+\infty$; z_0 is the coordinate of the graded-gap layer center; l_v is the length of graded-gap layer.

The task is to obtain dependences optimized by voltage of microwave generation efficiency on frequency for various lengths of the active region l_a and graded-gap layer l_v by numerical simulations. We have considered three different types of TED: $n^+ - n - n^+$, $n^+ - n^- - n - n^+$ and $n^+ - n^- - n^+ - n - n^+$. Fig. 1 shows the diagram of the conduction band and the distribution of InN in the $n^+ - n - n^+$ TED. The length l_a of the active region was 0.4, 0.8 and 2.5 µm with the concentration of ionized impurities n_0 in it equal to 10^{17} , $8{\cdot}10^{16}~\text{and}~3{\cdot}10^{16}\,\text{cm}^{-3},$ respectively. The concentration in the n^+ -region of $n^- - n^+$ -cathode was $8 \cdot 10^{16} \text{ cm}^{-3}$ $(l_a = 2.5 \ \mu\text{m})$ and $3 \cdot 10^{17} \text{ cm}^{-3}$ $(l_a \le 0.8 \ \mu\text{m})$, and in the n-region it was by the order lower than in the active one. The temperature of crystal lattice was considered constant and equal to 300 K.



Fig. 1. Schematic band diagram and the distribution of *x* binary component in the graded-gap $Al_{1-x}In_xN$ TED: $\boldsymbol{\varepsilon}_0$ is the energy level of vacuum; $\boldsymbol{\varepsilon}_l$ – vacuum level in the presence of external forces (local level); $\boldsymbol{\varepsilon}_C$ – bottom of conduction band (the energy minimum of the Γ -valley); $\boldsymbol{\varepsilon}_F$ – Fermi energy level; $\boldsymbol{\varepsilon}_V$ – valence band top; $\boldsymbol{\varepsilon}_g$ – forbidden band width; Γ , *U* and *A* are the energy minimum of the Γ -, *U*- and *A*-valleys; χ is the energy of the electron affinity; φ – potential of external forces; *z* – spatial coordinate; l_c , l_a and l_v are the lengths of cathode, active zone and graded-gap layer, respectively.

3. Experimental

The research has been carried out using the three-level model of IET in the graded-gap semiconductors based on the solution of the Boltzmann equation for the case of a displaced Maxwellian distribution for electrons [13]. This model represents a system of equations consisting of continuity equations (2), the current density equations (3) and the energy balance equations (4) for each of the three non-equivalent valleys of the semiconductor conduction band, as well as the Poisson equations (5):

$$\frac{\partial n_i}{\partial t} = -\frac{1}{e} \frac{\partial j_i}{\partial z} - \frac{n_i}{\tau_{n,ij}} - \frac{n_i}{\tau_{n,i\kappa}} + \frac{n_j}{\tau'_{n,ji}} + \frac{n_\kappa}{\tau'_{n,\kappa i}}; \qquad (2)$$

$$j_i = n_i \mu_i \left(eE + \frac{\partial \chi_i}{\partial z} \right) + \kappa_{\rm B} \mu_i \left(\frac{3n_i T_i}{2m_i} \frac{\partial m_i}{\partial z} - \frac{\partial (n_i T_i)}{\partial z} \right), (3)$$

$$\frac{3}{2}\kappa_{\rm B}\frac{\partial n_i T_i}{\partial t} = j_i E + \frac{j_i}{e}\frac{\partial \chi_i}{\partial z} - \frac{5}{2}\kappa_{\rm B}\frac{1}{e}\frac{\partial (j_i T_i)}{\partial z} - \frac{3}{2}\kappa_{\rm B}\left(\frac{n_j T_j}{\tau'_{{\rm E},ji}} + \frac{n_{\kappa} T_{\kappa}}{\tau'_{{\rm E},\kappa i}} - \frac{n_i T_i}{\tau_{{\rm E},i}}\right),$$
(4)

$$\frac{\partial(\varepsilon E)}{\partial z} = 4\pi e \left(n_i + n_j + n_\kappa - n_0 \right), \tag{5}$$

where the indices i, j and κ determine the three nonequivalent valleys. Eqs (2)-(4) are written down for the *i*-th valley. n_i , μ_i , m_i , j_i , T_i are the concentration, mobility, effective mass, current density and electron temperature in the *i*-th valley, respectively; $\tau_{n,ij}$, $\tau_{E,ij}$ are the relaxation time of concentration and energy of electrons during the intervalley transition from *i*-th to *j*-th valley; $\tau_{E,i}$ is the energy relaxation time of electrons in the *i*-th valley; χ_i is the energy, which is necessary to transfer electrons from the minimum energy level of the *i*-th valley to the local vacuum level; E is the electric field, n_0 is the concentration of ionized donors; ε is the dielectric permittivity; e is the absolute value of electron charge; $\kappa_{\rm B}$ is the Boltzmann constant; t is time; z is a coordinate. The average current density in the diode is defined as the sum of the averages in the three valleys. Γ , A and U energy minima were taken into account in our calculations [1, 8]. The system of Eqs (2)-(5) was solved numerically. The situation was simulated when the sinusoidal voltage with a constant component was applied to the diode, which corresponds to placing the diode into the single-loop resonator. The output performances were optimized for different frequencies with respect to the bias voltage and the amplitude of the first harmonic. The computation of the generation efficiency of the diodes was carried out for the second and third periods of oscillations.

4. Results and discussions

In the graded-gap AlInN TED, the mode with growing space-charge waves, i.e. domains, is realized independently of the doping profile in contrast to that in InN TED $n^+ - n - n^+$ -structure, where accumulation

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layers are formed. In general, operation of different types of TED based on graded-gap AlInN is determined by the same features as operation of TED based on InN and AlN binary nitrides [8]. It should be noted that at the selected doping level the linear dimensions of the formed domain are larger than the active region dimensions. Moreover, the domains penetrate into the anode at the depth of the order of 100 nm, which leads to the shift of the optimal generation frequency towards the lower frequencies. The same deficiency is typical for AlN and InN diodes.

The feature of the TED based on graded-gap semiconductors is the dependence of the output performances on the rate of changing the binary component percentage, which in this case is determined by the length of the graded-gap layer l_{ν} . The dependences of peak values of generation efficiency on the l_{ν} of different types of TED possess optima (Fig. 2).

The optimal length of graded-gap layer, at which the efficiency is maximum, depends on the type of the cathode contact as well as on the length of the active region and the concentration of ionized impurities in it. The feature of the TED based on graded-gap AlInN is that the optimal length of graded-gap layer is less than that of the active region (Table 1) as compared to AlGaAs and InGaAs [14, 15], where the optimal length of graded-gap layer is approximately equal to the length of the active region.

Table 1. Optimum graded-gap Al_{1-x}In_xN layer length.

	Active region length, µm				
Cathode type	2.5	0.8	0.4		
	Graded-gap AlInN layer length, µm				
n^+ - n - n^+	0.63	0.26	0.20		
$n^{+}-n^{-}-n-n^{+}$	0.80	0.35	0.30		
$n^{+}-n^{-}-n^{+}-n-n^{+}$	0.72	0.33	0.30		



Fig. 2. Dependence of generation efficiency peak values for AlInN TED on the length of graded-gap layer at the different length of active region: $0.4 \,\mu m$ (*1*); 0.8 (2); 2.5 (3). The solid curves correspond to the $n^+ - n^- - n - n^+$ TED, the dashed curves relate to the $n^+ - n - n^+$ TED.

The length of the graded-gap layer l_v also has impact on the optimal frequency of TED generation f_0 . With decreasing the l_v , a slight increase in f_0 occurs. For example, in $n^+ - n - n^+$ TED with $l_a = 2.5 \ \mu\text{m}$ when the l_v changes from 0.3 to 3 μm , f_0 increases from 68 up to 72 GHz. In the same diode, but with $l_a = 0.8 \ \mu\text{m}$ when the l_v changes from 0.1 to 1 μm , f_0 increases from 199 up to 223 GHz. In the TED with a high-ohmic heterogeneity $(n^+ - n^- - \text{ and } n^+ - n^- - n^+ - \text{cathode}), \ l_v$ impact on the output performances is weaker.

 n^+ - n^- -n- n^+ TED possesses the largest peak efficiency values. n^+ - n^- - n^+ -n- n^+ and n^+ -n- n^+ TED possess slightly lower peak values. For all the TED types, the maximum generation efficiency decreases with reduction of the active region length (Fig. 3, Table 2). Significant reduction in efficiency occurs when l_a becomes less than 0.6...0.8 µm. Efficiency peak values of similar devices for 0.8 and 2.5 µm lengths are almost identical. This is related to good inertial properties of AlN and InN.

Dependences of generation efficiency on the frequency of different InN diodes are shown in Fig. 4. They are similar to the performances obtained in [8] using the two-level model of IET effect.

Our comparative analysis of InN and graded-gap AlInN diodes shows that the AlInN TED exceeds similar devices based on InN, depending on the length and type of cathode in its efficiency by 1.11...2.32 times and by the output power by 1.36...1.95 times. Power consumption in AlInN diodes is by 0.80...1.29 times larger than in InN diodes. Moreover, the reduction of power consumption by 3...20% takes place only in the diodes of $n^+ - n^- - n - n^+$ and $n^+ - n^- - n^+ - n - n^+$ structures when $l_a \leq 0.8 \ \mu\text{m}$. It should be noted that TEDs based on semiconductor nitrides have high, as compared to GaAs, values of the output power (Table 3), which was also mentioned in publications [6, 10].



Fig. 3. Dependences of the efficiency on the frequency of AlInN diodes at the optimum graded-gap layer length and different active region length: $0.4 \ \mu m (1)$; 0.8 (2); 2.5 (3). The solid curves correspond to the $n^+ - n^- - n - n^+$; the dashed curves relate to the $n^+ - n^- - n^+$; the dash-dotted curves correspond to $n^+ - n^- - n^+$ and n^+ diodes.

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Fig. 4. Dependences of the efficiency on the frequency of InN diodes at different active region length: $0.4 \ \mu m(1)$; 0.8(2); 2.5(3). The solid curves correspond to the $n^+ - n^- - n - n^+$; the dashed curves relate to the $n^+ - n - n^+$; the dash-dotted curves correspond to $n^+ - n^- - n^+ - n - n^+$ diodes.

The optimal generation frequency for InN diodes is 22% higher than for graded-gap AlInN diodes.

The performances of AlN TED (Table 2 and 3) within the considered frequency range concede to AlInN and InN TED in the efficiency, output power and power consumption, as well as optimal frequency generation.

Graded-gap TEDs have one feature more: the length of drift region of the charge instability in the graded-gap layer depends on the voltage applied to the diode [16]. When the voltage applied to the diode is increased, the length of drift region extends and the oscillation frequency of current decreases. The manifestation of this effect can be seen in the $n^+ - n - n^+$ -diodes through the increasing high-frequency limit of the dependence of efficiency on frequency (Fig. 3). $\eta(f)$ plots are not symmetric with respect to the optimum frequency f_0 . The optimum supply voltage decreases when the frequency is increased.

Table 2. Maximum efficiency and the correspondinggeneration frequency for graded-gap AlInN, InN and AINTED.

Cathada	Active region length, µm							
type	2.5		0.8		0.4			
	η, %	f, GHz	η, %	f, GHz	η, %	f, GHz		
Al _{1-x} In _x N								
n^+	6.4	70	5.9	220	3.49	440		
n^+ - n^-	7.3	60	7.1	190	5.70	370		
$n^{+}-n^{-}-n^{+}$	5.7	58	5.6	185	4.81	390		
InN								
n^+	3.5	85	2.7	277	1.54	540		
n^+ - n^-	5.9	77	5.1	225	3.06	480		
$n^{+}-n^{-}-n^{+}$	5.1	68	3.0	275	2.07	480		
AlN								
n^+	1.1	38	0.81	120	0.6	205		
n^+ - n^-	1.5	34	1.3	115	1.0	200		

Table 3. The output power of graded-gap AlInN, InN and AlN TED.

	1					
	Active region length, µm					
Cathode	2.5	0.8	0.4			
type	W					
	W⋅cm ⁻²					
Al _{1-x} In _x N						
n^+	$8.3 \cdot 10^5$	$6.3 \cdot 10^5$	$2.0 \cdot 10^5$			
n^+ - n^-	$11.3 \cdot 10^5$	$10.5 \cdot 10^5$	$4.1 \cdot 10^5$			
$n^{+}-n^{-}-n^{+}$	$8.2 \cdot 10^5$	$8.1 \cdot 10^5$	$4.5 \cdot 10^5$			
InN						
n^+	$4.1 \cdot 10^5$	$4.6 \cdot 10^5$	$1.4 \cdot 10^5$			
n^+ - n^-	$7.4 \cdot 10^5$	$6.4 \cdot 10^5$	$2.2 \cdot 10^5$			
$n^{+}-n^{-}-n^{+}$	$5.86 \cdot 10^5$	$4.7 \cdot 10^5$	$2.3 \cdot 10^5$			
AIN						
n^+	$2.0.10^{5}$	$1.2 \cdot 10^5$	$1.1 \cdot 10^5$			
n^+-n^-	$2.7 \cdot 10^5$	$2.5 \cdot 10^5$	$1.6 \cdot 10^5$			

A similar effect takes place also in InN diodes with $n^+ - n^- - n - n^+$ -structure. However, it is caused by inhomogeneous distribution of electric field in the $n^- - n$ -contact.

Operation of graded-gap AlInN, InN and AlN diodes has also been considered in the biharmonic mode, when the voltage applied to the diode contains fundamental and second harmonics, which corresponds to placing a diode in a double-circuit resonator. When generating the fundamental harmonic in the double-circuit resonator, the generation efficiency and the output power are slightly increased. The relative increment in efficiency equals to 5...6%. Second harmonic generation is difficult because of large sizes of domains. Conditions, when there are two instabilities of the charge in the active region, have not been found yet. Therefore, we can assume that the second harmonic generation is possible in the frequency multiplication mode or in the mode of homogeneous field.

The estimations, made for graded-gap AlInNdiodes with $l_a = 0.2 \,\mu\text{m}$ as well as the dependence of efficiency on the active region length and frequency, show that the minimum active region length is about 0.15 μ m and maximum operation frequency is 0.9...1.3 THz. The minimum active region length of InN diodes is about 0.35 μ m, and the maximum frequency is 0.7...0.8 THz.

5. Conclusions

- 1. The graded-gap AlInN TEDs, the composition of which is changed from AlN to InN in the active region, can efficiently operate in the microwave frequency generation mode up to 0.9...1.3 THz. For the similar InN-diodes, the frequency limit is 0.7...0.8 THz.
- 2. The optimal length of the graded-gap AlInN layer, depending on the active region length and the doping profile, lies within the range 0.2 to $0.8 \,\mu\text{m}$.

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The diode has the maximum peak values of efficiency and output power at the optimal length of the graded-gap layer.

- 3. The graded-gap AlInN TEDs exceed the InN TEDs of the same type with respect to the generation efficiency and output power, but concede to them in the optimal generation frequency. The power consumption of AlInN-diodes with high-ohmic heterogeneity at the cathode and active region length less than $0.8 \ \mu m$ is by 3...20% less than in the InN diodes of the same type.
- 4. Within the considered frequency range AlN diodes concede to InN and graded-gap AlInN TEDs in the efficiency, output power and power consumption, as well as in the optimal generation frequency.
- 5. When the fundamental harmonic is generated in the double-circuit resonator, the relative increment of generation efficiency and output power is 5...6%. Second harmonic generation is difficult because of large sizes of domains. Second harmonic generation is possible in the frequency multiplication mode or in the mode of homogeneous field.

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