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A CHAOTIC POTENTIAL OF CHARGED DISLOCATIONS IN GROUP III-NITRIDE HETEROJUNCTIONS DURING LOCALIZATION OF A TWO-DIMENSIONAL ELECTRON GAS

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Abstract. This work studies a chaotic potential (CP) in the heterojunctions of III-nitrides, the CP caused by the electrostatic field of charged dislocations, under localization conditions of a two-dimensional electron gas in the near-contact region. Within the framework of the statistical analysis of a Poisson ensemble of linear defects, the amplitude and scale of the CP in the contact plane have been determined. The CP parameter dependence on the density of surface states and the concentration of dislocations at the mobility threshold of the two-dimensional electron gas was shown. The CP amplitude was established to exceed 100 meV in a wide range of changes in the system parameters, in the presence of electronic charge localization effects in the heterojunctions.

Keywords: chaotic potential, III-nitride heterojunction, two-dimensional electron gas, natural size effect

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ХАОТИЧЕСКИЙ ПОТЕНЦИАЛ ЗАРЯЖЕННЫХ ДИСЛОКАЦИЙ В ГЕТЕРОКОНТАКТАХ III-НИТРИДОВ ПРИ ЛОКАЛИЗАЦИИ ДВУМЕРНОГО ЭЛЕКТРОННОГО ГАЗА

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Аннотация. В работе исследуется хаотический потенциал (ХП) в гетероконтактах III-нитридов, обусловленный электростатическим полем заряженных дислокаций, в условиях локализации двумерного электронного газа в приконтактной области. В рамках статистического анализа пуассоновского ансамбля линейных дефектов определены амплитуда и масштаб ХП в плоскости контакта. Показана зависимость параметров ХП от плотности поверхностных состояний и концентрации дислокаций на пороге подвижности двумерного электронного газа. Установлено, что при наличии эффектов

локализации электронного заряда в гетероконтактах амплитуда ХП превышает 100 мэВ в широком диапазоне изменения параметров системы.

Ключевые слова: хаотический потенциал, гетероконтакт III-нитридов, двумерный электронный газ, естественный размерный эффект

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Introduction

Two-dimensional electron gas (2DEG) generally has high mobility in heterojunctions based on III-nitrides. However, this property of the system considerably depends on the defect concentration in semiconductor structures. The defect concentration of the contacting semiconductors and the interface limits the mobility of free charge carriers [1]. In some cases, the mean free path of charge carriers can also be decreased as a result of their scattering by charged dislocations [1–3]. Evidently, studies into this type of processes should take into account both the possible concentrations of these extended defects in heterojunctions and the population of dislocation states [4]. The redistribution of electron density between the surface states and the linear defect states leads to changes in the electric field and potential in the junction plane. At certain threshold values of random fields, a state of strong localization of 2DEG may occur [5].

Estimates indicate that fluctuations in electric fields on the surface of semiconductors and the formation of chaotic potential (CP) can be associated not only with the defect concentration of the surface itself, but also with localized charges in the near-surface depletion layers. A classical size effect occurs in heterojunctions of semiconductor structures with a wide range of parameters, associated with the naturally commensurable characteristic scales in the space-charge region of a semiconductor [6]. It was found that an increase in the amplitude and characteristic scale of CP occurs under the conditions of this size effect and the inhomogeneity of the local fields of charged defects in heterojunctions with a decrease in the density of delocalized surface states [7]. Furthermore, the actual distribution of the electron charge in the junction region self-consistently depends on the CP formed at the interface, since the spectrum of surface states and possibly their localization change. In view of the weakened screening effect of localized 2DEG, it seems important to investigate the CP structures of charged dislocations in heterojunctions of nitride semiconductors.

The goal of this study is to determine the given CP in heterojunctions of III-nitrides and the nature of its dependence on system parameters.

Distribution of charged dislocation potential in a heterojunction

For example, let us analyze the heterostructure based on the AlGaN/GaN heterojunctions [8]. Consider a model where threading of misfit dislocations with a surface concentration N_{disl} in the given heterostructure is represented as charged defects oriented normal to the junction plane. If we neglect the interaction between dislocations, their number distribution can be assumed to be Poissonian. The probability that N of the given linear defects are located in the junction region of radius R in this representation is equal to

$$p(N) = \frac{< N >^N \exp(- < N >)}{N!}, \quad (1)$$

where $<N>$ is the average number of these defects in a given region, and $N_{disl} = \pi R^2$.

Due to the polarity of the chemical bond in aluminum and gallium nitride crystals, a piezoelectric effect and spontaneous polarization occur in mechanically stressed heterojunctions [8]. As a result of injection of electrons into the junction region, a surface field and corresponding band bending are formed in gallium nitride, while the magnitude of the latter exceeds half the band gap (about 1.8 eV). Since the formed channel layer of the considered heterostructure almost always contains undoped or compensated gallium nitride (GaN), the space charge in the region of band bending is mainly produced by charged dislocations. In the presence of large band bending, such extended defects within the space-charge regions are assumed to be uniformly charged with a certain linear density λ. If there is only a localized surface charge in the heterojunction, then it is possible to use the superposition principle to determine the parameters of the CP. It can be proved that in this case, the dominant contribution to large-scale fluctuations of the field in the junction is made by a system of charged dislocations [7].

The potential of the field of an arbitrarily selected dislocation in the junction plane is determined in the polar coordinate system, where ρ is the radial coordinate determining the distance from this linear defect to the observation point. Integration along a charged dislocation within the space-charge region of width L_0 gives the potential energy of the surface electron in the junction plane:

$$U_i(\rho) = \frac{2e\lambda}{\varepsilon_1 + \varepsilon_2} \ln \frac{\sqrt{\rho^2 + L_0^2} + L_0}{\rho}, \tag{2}$$

where ε_1, ε_2 are the values of the dielectric constant of the semiconductors brought into contact.

The volume charge in the band bending region of GaN has a density equal to λN_{disl} within the model representations given above. In this case, the characteristic width of the space-charge region can be represented as

$$L_0 = \sqrt{\frac{\varepsilon_2 U_0}{2\pi e \lambda N_{disl}}}, \tag{3}$$

where U_0 is the band bending.

Simple calculations similar to those in [7] are necessary for further analysis of the system. First, the average contribution to the potential energy of the surface electron in the electric field of a single dislocation can be determined within the framework of the given method. Similar averaging of expression (2) over an area with radius yields the following result:

$$< U_i > (R) = \frac{2e\lambda}{(\varepsilon_1 + \varepsilon_2) R^2} \left(L_0 \sqrt{R^2 + L_0^2} - L_0^2 + R^2 \ln \frac{\sqrt{R^2 + L_0^2} + L_0}{R} \right). \tag{4}$$

Taking into account the distribution of charged dislocations (1), we can also represent the standard deviation of their number on the given surface region as

$$\delta N(R) = R\sqrt{\pi N_{disl}}. \tag{5}$$

Multiplying expressions (4) and (5), followed by a search for the maximum of the resulting product, we can estimate the characteristic magnitude of the inhomogeneities in the potential energy of the surface electron in the field of charged dislocations. The corresponding passage to the limit $R \to \infty$ gives the required value:

$$\delta U = \frac{4e\lambda L_0 \sqrt{\pi N_{disl}}}{\varepsilon_1 + \varepsilon_2}. \tag{6}$$

Substituting dependence (3) of the width of the space-charge region on the system parameters into expression (6), we obtain the following result:

$$\delta U = \frac{2}{\varepsilon_1 + \varepsilon_2} \sqrt{2e\lambda\varepsilon_2 U_0}. \tag{7}$$

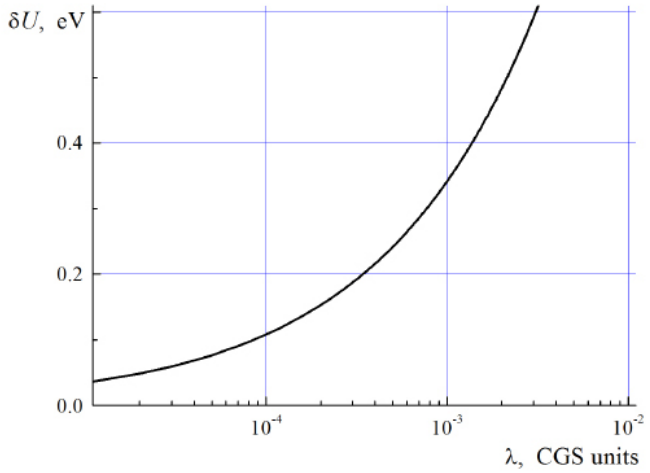

Fig. 1. Dependence of the average fluctuations in the chaotic potential of charged dislocations in the AlGaN/GaN heterojunction on the linear charge density. The band bending U_0 = 1.8 eV

The dielectric permittivities of aluminum nitride and gallium nitride in the considered heterostructure are 9.2 and 10.4, respectively [8]. The characteristic form of the obtained dependence $\delta U(\lambda)$ (see Eq. (7)) is shown in Fig. 1 for the value of band bending parameter U_0 = 1.8 eV. Since expression (6) for δU was obtained with a formal passage to the limit $R \to \infty$, the CP found in this manner is large-scale.

Density of surface states in the heterojunction

The presence of large-scale CP of charged dislocations in the near-contact region of the heterostructure under consideration modifies the quasi-classical spectrum of surface states and leads to the appearance of 'tails' in their density. In this case, with the known form of the law for the distribution of the potential energy of the electron, we can obtain the corresponding energy dependence of the density of states $D(E)$ [9]. In view of the quasi-continuity of the spectrum of electron states, the initial expression for their density takes the form

$$D(E) = \int_{-\infty}^{E} D_0(E-U) \cdot f(U)\, dU, \tag{8}$$

where $D_0(E)$ is the unperturbed density of states, $f(U)$ is the probability density function for the potential energy of the electron U on the surface.

The quasi-classical density of surface states for parabolic dispersion is constant within the allowed band in the absence of CP and valley degeneracy [10], depending only on the effective electron mass. Therefore, expression (8) can be simplified:

$$D(E) = D_0 \int_{-\infty}^{E} f(U)\, dU. \tag{9}$$

Thus, the type of functional dependence $D = D(E)$ is completely determined by the nature of the potential energy distribution of the surface electron. The Gaussian model of CP distribution is adequate for taking into account the superposition of fields of randomly located charged dislocations [11]:

$$f(U) = \frac{1}{\delta U \sqrt{2\pi}} \cdot \exp\left(-\frac{U^2}{2 \cdot \delta U^2}\right). \tag{10}$$

After substituting probability density function (10) into expression (9) and calculating the integral, we obtain the density of surface states in terms of the error function:

$$D(E) = \frac{D_0}{2} \cdot \left[1 + erf\left(\frac{E}{\delta U \sqrt{2}} \right) \right]. \quad (11)$$

This formula allows to obtain the expression for the concentration of 2DEG

$$n_S = \int_{-\infty}^{E_F} D(E)\, dE, \quad (12)$$

at low temperatures T (formally at $T \to 0$ K), which has the following form [12]:

$$n_S = \frac{D_0}{2} \cdot \left\{ E_F \left[1 + erf\left(\frac{E_F}{\delta U \sqrt{2}} \right) \right] + \delta U \sqrt{\frac{2}{\pi}} \exp\left(-\frac{E_F^2}{2 \cdot \delta U^2} \right) \right\}. \quad (13)$$

Here E_F is the Fermi energy in the surface zone.

Chaotic potential in the heterojunction at the mobility threshold of two-dimensional electron gas

The specific values of the quantities δU and n_S can be estimated under known conditions characteristic of the contacting structures formed. First of all, it can be assumed that the electroneutrality condition is satisfied in the equilibrium state:

$$N_S = n_S + \frac{\lambda}{e} N_{disl} L_0, \quad (14)$$

where N_S is the surface charge density in the junction.

If quantity (14) depends only on the nature of the contacting semiconductors, then $N_S = const$ for the given heterostructure. In this case, only the redistribution of localized charge between the surface and dislocation states is possible, depending on the specific scenario. For example, almost all localized surface states are filled at the classical mobility threshold (i.e., provided that $E_F = 0$ [9]), which corresponds to the condition that the maximum electron charge appear on the dielectric surface. In this case, an explicit dependence of the characteristic values of CP on the number of charged dislocations per unit surface area of the junction can be obtained from expression (14) in view of (3), (7) and (13)

$$\delta U = \frac{4\sqrt{2\pi} \cdot e^2 N_S}{4e^2 D_0 + (\varepsilon_1 + \varepsilon_2)\sqrt{2N_{disl}}}. \quad (15)$$

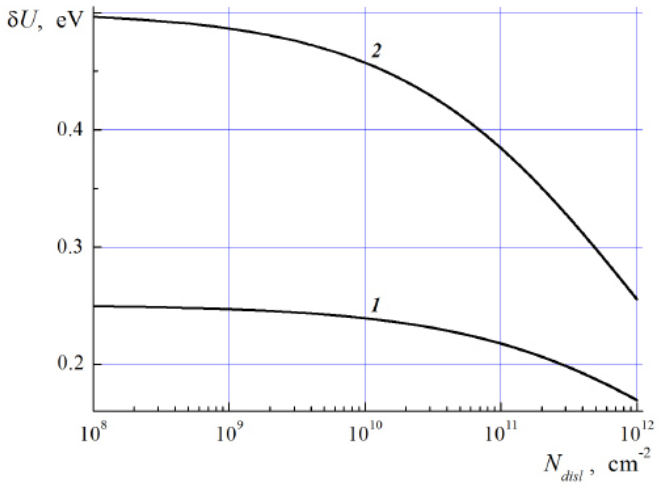

Fig. 2. Dependences of the average fluctuations in the chaotic potential of charged dislocations in the heterojunction on their concentration at the mobility threshold of two-dimensional electron gas, at two surface state densities D_0, $cm^{-2} \cdot eV^{-1}$: $1 \cdot 10^{14}$ (*1*) and $5 \cdot 10^{13}$ (*2*); $N_S = const$

The dependence of the average potential energy fluctuations (15) on the concentration of charged dislocations for the surface charge density $N_S = 10^{13}$ cm^{-2} and two densities of surface states D_0 is shown in Fig. 2.

Results and discussion

Analysis shows that the amplitude of CP in the heterojunction for localized 2DEG can reach several hundred millielectronvolts (see Fig. 1) even at fairly moderate values of the linear charge density in dislocations (compared with the maximum possible values of the order of 0.01 CGE units [7]). The dependence $\delta U = \delta U(\lambda)$ obtained for this case is rather weak: according to expression (7), the quantity δU is proportional to the square root of the linear charge density λ. In other words, the indicated values of the characteristic inhomogeneities of the potential in the junction are preserved in a fairly wide variation range of the system parameters. Moreover, due to the presence of unscreened Coulomb fields of form (2), slowly varying in space, the resulting CP in the junction turns out to be large-scale.

The natural consequences of the existence of large-scale CP in the heterojunction are the appearance of 'tails' in the density of surface states and the possibility of redistribution of localized charge. If the total surface charge remains unchanged in the heterojunction, then the average value of fluctuations in the potential energy of the surface electron decreases with an increase in the charged dislocation concentration within the framework of the model approximation adopted (see Fig. 2). This behavior of the quantity δU is associated with a weakening of the intrinsic size effect, since in this case the charge is distributed over a larger number of extended defects and better statistical averaging of inhomogeneous fields is achieved. A decrease in the density of surface states (which corresponds to lower effective electron masses in the surface zone) leads to a noticeable increase in δU.

Conclusion

The paper reports on the behavior of the chaotic potential (CP) in III-nitride heterojunctions, induced by the electrostatic field of dislocations for localized two-dimensional electron gas in the near-contact region. The amplitude of the CP in the junction plane and the nature of the spatial distribution of the corresponding field are determined. The dependence of the characteristic values of CP on the system parameters is considered. It is established that the magnitude of CP amplitude can exceed 100 MeV in the presence of electron charge localization effects in III-nitride heterojunctions. This result is important both from the standpoint of improving the technology for synthesis of semiconductor devices based the corresponding heterostructuctures, and from the standpoint of theoretical studies into the properties of two-dimensional electron gas.

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