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A CHAOTIC POTENTIAL OF CHARGED DISLOCATIONS IN THE III-NITRIDE HETEROJUNCTIONS AT HIGH TEMPERATURES

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Abstract. The paper studies the high-temperature structure of a chaotic potential (CP) induced in heterojunctions of the group III nitrides by the electrostatic field of charged dislocations. The CP amplitude in the junction plane has been obtained taking into account the spatial dispersion of a dielectric response of two-dimensional electron gas. The dependence of the CP properties on the parameters of the system was found. In particular, the magnitude of the CP amplitude exceeds that of the thermal energy, if the two-dimensional non-degenerate gas given in III-nitride heterojunctions and the dislocation densities being up to and over 10^{10} cm^{-2}.

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

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ХАОТИЧЕСКИЙ ПОТЕНЦИАЛ ЗАРЯЖЕННЫХ ДИСЛОКАЦИЙ В ГЕТЕРОКОНТАКТАХ III-НИТРИДОВ ПРИ ВЫСОКИХ ТЕМПЕРАТУРАХ

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Аннотация. В работе исследуется высокотемпературная структура хаотического потенциала (ХП) в гетероконтактах III-нитридов, обусловленного электростатическим полем заряженных дислокаций. С учетом пространственной дисперсии диэлектрического отклика двумерного электронного газа определена амплитуда ХП в плоскости контакта. Показана зависимость свойств ХП от параметров системы. В частности, при наличии невырожденного двумерного электронного газа в гетероконтактах III-нитридов и плотности дислокаций 10^{10} см$^{-2}$ и более, величина амплитуды ХП превышает значение тепловой энергии.

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

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Introduction

Heterojunctions based on nitrides of Group III elements (Al, Ga, In) are finding increasing applications in solid-state devices used as high-power microwave sources [1]. While these systems offer a number of obvious advantages over the structures based on $A^{III}B^{V}$ compounds, certain drawbacks remain due to the specifics of the synthesis technology, affecting, for example, the parameters of high-electron-mobility transistors (HEMT) [2]. The parameter fluctuations detected for the devices are likely due to the initial defects in the materials and heterointerfaces forming. Lattice mismatch in III-nitrides and substrates used is known to generate initial misfit/threading dislocations, turning out to be electrically charged in many cases [3]. Electron scattering by charged dislocations in the 2D channel of the HEMT produces a certain decrease in electron mobility [4–7]. Moreover, the effect of this scattering can increase manifold at threshold values of the transmitted power, as the screening properties of the two-dimensional electron gas (2DEG) deteriorate at high temperatures, when this electronic subsystem ceases to be degenerate. The inhomogeneous field of charged dislocations is not averaged in these conditions, which means that fluctuations in the strength and chaotic potential are observed in the 2DEG plane. The interaction induced by the inhomogeneous electric field of the system of linearly distributed charges is in fact self-consistent, since it is primarily the density of surface states that has a finite magnitude. The chaotic potential causes tails to appear in the density of electronic states, with part of the carriers localized to the conducting channel in HEMT.

The goal of this study consisted in characterizing the chaotic potential of charged dislocations in heterojunctions of nitride semiconductor compounds at high temperatures.

Charged dislocation field

To be definite, we consider an indium-containing structure, InAlN/GaN [8], remaining stable at record high temperatures up to 1000 °C. Misfit dislocations with the surface density N_{disl} are represented by linear defects that are normally oriented to the junction plane. If the spatial arrangement of these extended defects is uncorrelated, their number follows a Poisson distribution with the parameter

$$\langle N \rangle = N_{disl} S$$

determining the mean number of these defects in the near-junction region with an area S.

Since the channel layer is formed from undoped (or compensated) GaN, the space charge in the near-junction region with band bending is generated primarily by charged dislocations. These extended defects within the space charge region can be assumed to be uniformly charged at large band bending, with a certain linear density taking the maximum value λ. If a delocalized surface charge is present in the heterojunction, the electrostatic image method can be used at a high density of surface states D_s (over 10^{14} cm^{-2}eV^{-1}) to establish the parameters of a chaotic field [9]. We determine the field of an arbitrarily chosen dislocation in a cylindrical coordinate system, where ρ is the radial coordinate measuring the distance from the dislocation in the junction plane. The magnitude of the field strength for a charged dislocation is obtained by a simple calculation in the form

$$F_i(\rho) = \frac{2\lambda}{\varepsilon}\left(\frac{1}{\rho} - \frac{1}{\sqrt{\rho^2 + L_0^2}}\right), \quad (1)$$

where ε is the dielectric constant of the medium where the ith dislocation is located, L_0 is the width of the space charge region.

Assuming that 2DEG is strongly degenerate, let us now turn to analysis of expression (1), focusing on the nature of the dislocation distribution. The mean value of (1) in an area of radius R is found from the expression

$$\langle F \rangle_i (R) = \frac{4\lambda}{\varepsilon R^2}\left(R - \sqrt{R^2 + L_0^2} + L_0\right). \quad (2)$$

As a matter of fact, Eq. (2) determines the mean contribution of one charged dislocation to the field strength. Considering the distribution of charged dislocations, we can also represent the mean fluctuations in their number in the corresponding surface region with an area $S = \pi R^2$ in the form

$$\delta N(R) = R\sqrt{\pi N_{\text{disl}}}. \tag{3}$$

The product of (2) by (3) gives an estimate for the characteristic scale of the inhomogeneities in the surface field strength

$$\delta F(R) = \frac{4\lambda}{\varepsilon R}\sqrt{\pi N_{\text{disl}}}\left(R - \sqrt{R^2 + L_0^2} + L_0\right). \tag{4}$$

The resulting function (4) is monotonically decreasing, reaching its maximum at $R << L_0$. Calculating the exact upper bound of this expression (in the limit $R \to 0$), we obtain the amplitude of the chaotic field:

$$\delta F = \frac{4\lambda\sqrt{\pi N_{disl}}}{\varepsilon}. \tag{5}$$

These high densities of surface states allow to directly estimate the magnitude of the chaotic potential amplitude in the 2DEG plane. The magnitude of potential inhomogeneities can be found under these conditions in the Thomas–Fermi approximation:

$$\delta\sigma = eD_s \cdot \delta U. \tag{6}$$

It is assumed here that the potential perturbation is small in comparison with the mean electron energy in the surface zone, while the variation in the density of states is neglected. Next, taking into account the linear dependence of the surface charge on the field strength $F = 4\pi\sigma/\varepsilon$, as well as expressions (5) and (6), we can relate the quantity δU with the parameters of the system:

$$\delta U = \frac{\lambda}{eD_s}\cdot\sqrt{\frac{N_{disl}}{\pi}}. \tag{7}$$

Case of low density of electron states

The case when the densities of electron states in a heterojunction are relatively low deserves more detailed analysis of the potential fluctuations emerging, using the dielectric response function of the surface subsystem. The potential energy of a surface electron in the field of a charged dislocation without a reaction of the medium takes the form

$$V_i(\rho) = e\lambda \cdot \ln\frac{\sqrt{\rho^2 + L_0^2} + \rho}{\rho}. \tag{8}$$

In view of the Fourier–Bessel transformation (8) [10] in the space of wave vectors q, we have

$$V_i(q) = \frac{e\lambda}{q^2}\cdot\left[1 - \exp(-qL_0)\right]. \tag{9}$$

The dielectric response function has the following form in the high-temperature region (i.e., for classical statistics of two-dimensional electron gas) [11]:

$$\varepsilon(q) = \frac{\varepsilon_1 + \varepsilon_2}{2}\cdot\left(1 + \frac{q_s(q)}{q}\right), \tag{10}$$

where ε_1 and ε_2 are the dielectric constants of contacting semiconductors, $q_s(q)$ is the screening parameter in a two-dimensional electronic system. The relation $q << q_s$ also holds true with large band bends for most of the harmonics; in this case, the dielectric response function (10) can be approximately represented as [12]:

$$\varepsilon(q) \approx \frac{2\pi e^2 n_s}{kT \cdot q}. \quad (11)$$

Using the form of the initial potential (9), the inverse Fourier–Bessel transform, and the expression for the dielectric response of system (11), we obtain the potential electron energy in the surface plane accounting for screening:

$$U_i(\rho) = \frac{\lambda kT}{2\pi e n_s} \cdot \left(\frac{1}{\rho} - \frac{1}{\sqrt{\rho^2 + L_0^2}} \right). \quad (12)$$

The functional dependence on the radial coordinate in (12) coincides with a similar dependence in (1), allowing to repeat the previous calculation algorithm for directly finding the amplitude of the chaotic potential:

$$\delta U = \frac{\lambda kT}{e n_s} \cdot \sqrt{\frac{N_{disl}}{\pi}}. \quad (13)$$

The resulting expression may not be final, requiring in some cases to additionally find the 2DEG density in terms of the chaotic potential parameters, i.e., to establish the functional dependency $n_s = n_s(\delta U)$.

The corresponding density of electron states $D(E)$ can be obtained for a specific form of the potential energy distribution for a surface electron, characterized by the probability density $p(U)$. Since the density of surface states is initially constant if dispersion follows a parabolic law, this density takes the following form in the presence of a chaotic potential [13]:

$$D(E) = D_s \int_{-\infty}^{E} p(U)\, dU, \quad (14)$$

Calculating the integral in (14) for a Gaussian distribution with the standard deviation parameter equal to δU yields the result known from probability theory via the error function:

$$D(E) = \frac{D_s}{2} \cdot \left[1 + erf\left(\frac{E}{\delta U \sqrt{2}} \right) \right]. \quad (15)$$

The density of 2DEG in the junction is determined by integration over all occupied states:

$$n_s = \int_{-\infty}^{+\infty} D(E) f(E)\, dE. \quad (16)$$

The Boltzmann distribution law

$$f(E) \approx exp[\mu - E)/kT]$$

should be chosen here for the high-temperature limit, where μ is the chemical potential measured from the bottom of the unperturbed surface band of electron states.

In view of the form that perturbed density (15) takes, we obtain from expression (16) [9]:

$$n_s = D_s kT \cdot \exp\left[\frac{\mu}{kT} + \frac{1}{2} \left(\frac{\delta U}{kT} \right)^2 \right]. \quad (17)$$

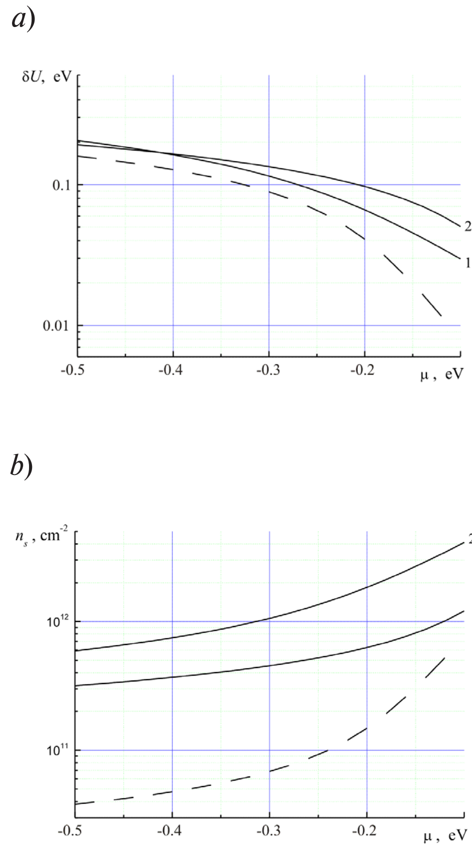

Fig. 1. Chaotic potential amplitude of charged dislocations (*a*) and 2DEG density (*b*) in a III-nitride heterojunction as functions of chemical potential for two temperatures, K: 600 K (curves *1* and dashes), 1200 K (*2*); $N_{\text{disl}} = 10^{10}$ cm^{-2} (*1*, *2*) and 10^8 cm^{-2} (dashes), $\lambda = 0.01$ ESU, $D_s \approx 10^{14}$ cm^{-2}eV^{-1}

Thus, to determine the magnitude of the chaotic potential amplitude, we should solve the transcendental equation obtained by substituting (17) into (13):

$$\delta U = \frac{\lambda}{eD_s} \cdot \sqrt{\frac{N_{disl}}{\pi}} \cdot \exp\left[-\frac{\mu}{kT} - \frac{1}{2}\left(\frac{\delta U}{kT}\right)^2 \right]. \tag{18}$$

The δU dependences calculated for the typical parameter values in the system are shown in Fig. 1.

Discussion

Summarizing the analysis carried out, we should note that the expression for the characteristic values of surface potential inhomogeneity at high temperatures (13) could be obtained from Eq. (7) by substituting the density of states D_s with the ratio n_s/kT. Estimating the values that δU takes for the chaotic potential parameters in heterojunctions based on III-nitrides, we adopt the effective electron mass in the surface zone $m^* \approx 0.2m$ (m is the electron rest mass) and the corresponding unperturbed density of surface states $D_s \approx 10^{14}$ cm^{-2}eV^{-1}. Then, assuming that the dislocation density at the interface is of the order of 10^{10} cm^{-2}, carrying the maximum charge per unit length of about 0.01 ESU, δU values in non-degenerate 2DEG exceed the thermal energies kT in a wide range of negative values of the chemical potential (or electrochemical potential, if a blocking voltage is applied to the transistor gate). The chaotic potential amplitude can reach over 100 meV in HEMP operating modes close to the cutoff, even at significantly lower dislocation densities (dashed line in Fig. 1). The corresponding 2DEG densities decrease from the initial levels (about 10^{13} cm^{-2}) by one or two orders of magnitude (Fig. 2).

Conclusion

We have considered the behavior of the chaotic potential induced in heterojunctions based on III-nitrides by the electrostatic field of the dislocations present throughout the material, carrying an electric charge. The CP amplitude in the junction plane at high temperatures has been determined taking into account the spatial dispersion of the dielectric response of two-dimensional electron gas. We have analyzed the dependence of the CP properties on the system parameters. Our main finding is that the CP amplitude exceeds the thermal energy level for non-degenerate 2DEG in III-nitride heterojunctions at dislocation densities of 10^{10} cm^{-2} or higher. This can lay the groundwork for future applications in semiconductor devices.

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