

## Electron States on the Rough GaAs (100) Surface, Formed by the Surface Acoustic Wave and Adsorbed Atoms

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The theory of electron states is developed on the adsorbed surface of semiconductor which is bounded by the rough surface. The surface roughness are formed by both quasi-Rayleigh acoustic wave and adsorbed atoms. A spectrum of surface electron states on the adsorbed surface of GaAs semiconductor in the long-wavelength, resonance and short-wave approximations is founded, taking into account the interaction of the first three electron harmonics under the action of an acoustic quasi-Rayleigh wave. It is shown that the dependences of the energy band gap width on the surface of the semiconductor and the length of the spatial localization of electron wave function on the adsorbed atoms concentration in the interval  $0 < N_{od} \leq 10^{13} \text{sm}^{-2}$  have the nonmonotonic character.

**Keywords:** Adsorbed atoms, Acoustic quasi-Rayleigh wave, Electron states.

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### 1. INTRODUCTION

Modern nanotechnologies allow to create the stress nanoheterosystems  $2D$ ,  $1D$ ,  $0D$ - dimensions and different geometric architectures, which are functional elements of nanoelectronics. However, the properties of such nanoheterosystems are determined largely by the quality of the heteroboundaries surface. Due to the fluctuation of structure of the epitaxial layers [1] and as a result of unconcordance of lattices parameters of contacting nanolayers [2], the subsurface layer and heteroboundary have the inhomogeneous relief. The presence of the latter leads to a deterioration of the transport characteristics of a two-dimensional electron gas in the subsurface layer of the semiconductor and nanoheterosystems. Therefore, the development of modern micro- and nanoelectrons needs the research of mechanisms of the electron states excitation on the surface and on the boundary of semiconductors. One of the mechanisms is the heterogeneous deformation of subsurface layer of semiconductor. This deformation is caused by both surface acoustic wave (SAW) and adsorbed atoms [3, 4].

At this time there are many works [5-7] which are dedicated to research of the surface quantum electron states. At the same time, the main attention was concentrated on the research of the electron states on the crystal surface, predetermined by the periodic crystal-line potential break. Depending on the choice of the physical model, there are Tamm surface states and Shockley states. The surface states of Tamm arise as a result of a change of the potential course on the crystal-vacuum boundary. The Shockley states are caused by the break atoms bonds on the boundary [8]. However, these two models do not cover all the tasks which would describe the arising of localized electronic states on the two media boundary division. It is known, if the surface is smooth the surface electronic states do not arise.

The surface electron states of semiconductor, lim-

ited uneven surface with an infinitely high potential barrier were investigate in the work [7]. The semiconductor surface was considered without adsorbed atoms, and the surface roughness were formed by quasi-Rayleigh acoustic wave.

Interaction between the adsorbed atoms and the acoustic quasi-Rayleigh wave, creating the dynamic deformation, renormalizes the spectrum of the surface electron states due to deformation potential. Changing technologically the adsorbed atoms concentration, it is possible to change the frequency of surface acoustic wave and the electronic structure of subsurface layer. Such correlation between the adsorbed atoms concentration and the frequency of surface acoustic wave can be used in practice for the change of coefficients of electromagnetic waves reflection from the interface of media and for the change of dispersion law of plasma oscillations.

In this work the conditions of arising of localized electron states on the semiconductor surface with roughness are theoretically investigated. These roughnesses are formed due to adsorbed atoms and acoustic quasi-Rayleigh wave.

### 2. FORMULATION OF THE PROBLEM

Let the atoms with an average concentration  $N_{od}$  are adsorbed in the subsurface layer of cubic crystal (GaAs, CdTe (100)) at the action of atoms flow in the molecular beam epitaxy or implantation process. Due to the deformation potential and the local renormalization of the surface energy, the adatoms and the deformation field of the surface acoustic quasi-Rayleigh wave deform inhomogeneously the subsurface layer. In turn, this inhomogeneous self-consistent deformation through the deformation potential redistributes adsorbed atoms along the surface. The influence of adsorbed atoms is reduced to a change of boundary conditions for a stress tensor  $\sigma_{ij}$  on  $z = 0$  surface. The defect-

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enriched subsurface layer can be considered as a film of a thickness,  $\rho$  density and Young's modulus  $E$ . It is connected rigidly with substrate – the other monocystal part with elastic parameters  $\rho_s$  and  $E_s$ . The connecting plane of film and substrate  $z = \alpha$  is parallel to the surface (100). The axis  $z$  is directed into the single crystal depth, the axes  $x$  and  $y$  – along two orthogonal crystallographic directions of type [100].

A surface acoustic quasi-Rayleigh wave, extending in  $x$  axis direction with  $\omega'(q, N_{od})$  frequency, forms the dynamic deformation and interacts with adatoms. The deformed surface form along the  $x$  axis, depending on time, can be described by the following function:

$$\omega'(q, N_{od}) = c_t q \xi_0 \left( 1 - \frac{1}{f'(\xi_0)} \frac{2\xi_0 \theta_d N_{od}}{k_B T \rho c_t^2} \cdot \frac{D_d^2 q (1 - \frac{2}{3} \frac{1-2\nu}{K(1-\nu)\alpha} \frac{\theta_d^2}{k_B T} N_{od}) q}{\left( D_d (1 - \frac{2}{3} \frac{1-2\nu}{K(1-\nu)\alpha} \frac{\theta_d^2}{k_B T} N_{od}) \right)^2 q^2 + c_t^2 \xi_0^2} (1 - l_d^2 q^2) \left( q \sqrt{1 - \xi_0^2} \frac{\partial F}{\partial N_{1d}} + (2 - \xi_0^2) \frac{\theta_d}{2\alpha} \right) \right) \quad (2)$$

$$\omega''(q, N_{od}) = \frac{c_t q}{f'(\xi_0)} \frac{2\xi_0^2 \theta_d N_{od}}{k_B T \rho c_t^2} \cdot \frac{D_d q}{\left( D_d (1 - \frac{2}{3} \frac{1-2\nu}{K(1-\nu)\alpha} \frac{\theta_d^2}{k_B T} N_{od}) \right)^2 q^2 + c_t^2 \xi_0^2} (1 - l_d^2 q^2) \left( q \sqrt{1 - \xi_0^2} \frac{\partial F}{\partial N_{1d}} + (2 - \xi_0^2) \frac{\theta_d}{2\alpha} \right) \quad (3)$$

where  $N_{od}$  is the spatially homogeneous component of adatoms concentration;  $K$  is the modulus of elasticity;  $l_d^2$  is the average of the square of characteristic distance of interaction between the adatom and the matrix atoms;  $\nu$  is the Poisson coefficient;  $\theta_d$  is the surface deformation potential;  $D_d$  is the diffusion coefficient of adatom;  $T$  is the temperature of substrate;  $k_B$  is the Boltzmann constant.

The height of the roughness  $\zeta(N_{od})$  is equal to the sum of the normal components of the displacement vector  $\vec{u}^l(\vec{r}, t)$ ,  $\vec{u}^t(\vec{r}, t)$  of longitudinal and transversal waves, respectively, on the plane  $z = 0$  [11]:

$$\zeta(N_{od}) = \left| \vec{u}_z^l(0) \right| + \left| \vec{u}_z^t(0) \right| \quad (4)$$

The components  $\vec{u}_z^l(0)$ ,  $\vec{u}_z^t(0)$  of the displacement vector of the medium points are founded from the equation solution [12]:

$$\frac{\partial^2 \vec{u}}{\partial t^2} = c_t^2 \Delta_r \vec{u} + (c_l^2 - c_t^2) \overline{\text{grad}(\text{div} \vec{u})} \quad (5)$$

The solution of equation (5) for the Rayleigh surface wave, extending in the  $x$  axis direction, is represented as:

$$u_x(x, z) = -iqAe^{iqx - i\omega t - k_t z} - ik_t B e^{iqx - i\omega t - k_t z}, \quad (6)$$

$$u_z(x, z) = k_t A e^{iqx - i\omega t - k_t z} + qB e^{iqx - i\omega t - k_t z}, \quad (7)$$

where  $k_{l,t}^2(N_{od}) = q^2 - \frac{\omega^2}{c_{l,t}^2}$ ;  $A, B$  – amplitudes of SAW.

$$\zeta(N_{od}) = k_t \sqrt{\alpha^3 \left/ \left( \frac{k_t}{2} \left( 1 - \frac{1}{e^2} \right) + \frac{k_t}{k_l + k_t} A \left( 1 - \frac{1}{e^{1+k_t/k_l}} \right) + \frac{q^2}{2k_t} B \left( 1 - \frac{1}{e^{2k_t/k_l}} \right) \right)} + 2q \sqrt{\alpha^3 B \left/ \left( \frac{k_t}{2} \left( 1 - \frac{1}{e^2} \right) + \frac{k_t}{k_l + k_t} A \left( 1 - \frac{1}{e^{1+k_t/k_l}} \right) + \frac{q^2}{2k_t} B \left( 1 - \frac{1}{e^{2k_t/k_l}} \right) \right)}$$

$$z_0(x, t) = \zeta(N_{od}) \cos(qx - \omega'(q, N_{od})t) \quad (1)$$

where  $q = \frac{2\pi}{L_x}$ ,  $L_x$  is period of roughness (length of acoustic wave) along the  $x$  axis.

It should be noted that the period of such roughness at frequency  $\omega'(q, N_{od}) \square 10$  GHz is 540 nm.

The dispersion law  $\omega'(q, N_{od}) = \text{Re} \omega$  of quasi-Rayleigh wave, renormalized by adatoms, and the width  $\omega''(q, N_{od}) = \text{Im} \omega$  of acoustic phonon mode are determined [9, 10]:

The deformation potential created by the surfaceacoustic quasi-Rayleigh wave and adsorbed atoms is determined by the following relation

$$V(x, z, t) = \lambda_{ij} \frac{\partial u_i(x, z, t)}{\partial x_j} \quad (8)$$

where  $u_i = u_i^l + u_i^t$ ;  $\lambda_{ij}$  is a tensor of deformation potential. The double indexes in formula (8) mean the summation.

The tensor of the deformation potential is taken in the form  $\lambda_{ij} = \lambda \delta_{ij}$ . Then, taking into account the last, formula (8) will look like

$$V(x, z, t) = \lambda \sum_i \frac{\partial u_i(x, z, t)}{\partial x_i} \quad (9)$$

Substituting in (9) the components of the displacement vector  $u_i(x, z, t)$  (4), (5), we obtain

$$V(x, z, t) = V_0 e^{-k_t z} e^{ikx - i\omega t} \quad (10)$$

where  $V_0 = -\frac{|\lambda| \zeta(N_{od}) q^2 (2 - \xi_0) \frac{c_t^2}{k_l}}{k_l \frac{c_t^2}{k_l}}$ ,  $\frac{1}{k_l}$  is the depth

of sound penetration in semiconductor,  $\xi_0$  is a quantity depended on the ratio between the longitudinal  $c_l$  and transversal  $c_t$  sound velocity [12].

Taking into account the relations (4), (6), (7) the expression for the roughness height  $\zeta(N_{od})$  will take the form [10]

$$A = \frac{-k_l^2 + (1-2\beta)q^2 + M}{\beta k_l}; \quad B = \frac{(-k_l^2 + (1-2\beta)q^2 + M)^2 + Z^2}{(2\beta k_l q)^2};$$

$$M = M(q, N_{0d}) = -\frac{\omega^2(q, N_{0d})}{c_l^2} \frac{\theta_d^2}{\rho c_l^2 a} \frac{D_d^2 N_{0d}}{D_d^2 q^4 + \omega^2(q, N_{0d})} \frac{q^2}{k_B T} (1 - l_d^2 q^2)$$

$$Z = Z(q, N_{0d}) = -\frac{\omega^3(q, N_{0d})}{c_l^2} \frac{\theta_d^2}{\rho c_l^2 a} \frac{D_d N_{0d}}{D_d^2 q^4 + \omega^2(q, N_{0d})} \frac{q^2}{k_B T} (1 - l_d^2 q^2)$$

The surface electron states on the rough boundary of semiconductor are founded from the non-stationary Schrodinger equation

$$i\hbar \frac{\partial \psi(x, z, t)}{\partial t} = -\frac{\hbar^2}{2m^*} \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V_0 e^{-k_l z} e^{ik_x - i\omega t} \psi(x, z, t) \quad (11)$$

The surface roughness are formed by a surface acoustic wave, which selfconsistently interacts with adsorbed atoms with concentration  $N_{0d}$ . The interaction between the surface acoustic wave and adsorbed atoms is formed through the deformation potential. We assume that the motion of conduction electrons is bounded by an uneven wall, which is an infinitely high potential barrier.

We find the solution of equation (11) as the sum of the space-time harmonics [7]:

$$\psi(x, z, t) = \sum_{n=-\infty}^{\infty} \psi_n(z) e^{i\Phi_n(x, t)}, \quad (12)$$

where  $n$  is a number of harmonic;  $\Phi_n(x, t) = (k_x + nq)x - (\omega_e + n\omega'(q, N_{0d}))t$ ;  $\hbar\omega_e = E$  is the electron energy;  $\hbar k_x$  is its impulse.

Substituting (12) into equation (11), we obtain:

$$\sum_{n=-\infty}^{\infty} \left( k_n^2 + \frac{\partial^2}{\partial y^2} \right) \psi_n(z) e^{i\Phi_n(x, t)} = -2\beta^2 q \tilde{\zeta}(N_{0d}) e^{-k_l z} \times \sum_{n=-\infty}^{\infty} \psi_n(z) e^{i\Phi_n(x, t)} \cos(qx - \omega'(q, N_{0d})t), \quad (13)$$

where  $k_n^2 = \frac{2m^*}{\hbar^2} (E + n\hbar\omega'(q, N_{0d})) - (k_x + nq)^2$ ,

$\beta^2 = \frac{m^* |V_0|}{\hbar^2 \tilde{\zeta}(N_{0d}) q}$ ;  $m^*$  - effective electron mass.

Multiplying the left and the right parts of equation (13) on a complex conjugate function  $e^{-i\Phi_m(x, t)}$  and using the condition of the functions orthogonality, we obtain:

$$\left( k_n^2 + \frac{\partial^2}{\partial y^2} \right) \psi_n(z) = -2\beta^2 q \tilde{\zeta}(N_{0d}) e^{-k_l z} (\psi_{n+1}(z) + \psi_{n-1}(z)), \quad (14)$$

Equation (14) is solved by the method of successive approximations for a small parameter  $q\tilde{\zeta}(N_{0d}) \ll 1$ . In the zero approximation the wave function  $\psi_n^0(z)$  will have the form:

$$\psi_n^0(z) = A_n e^{ik_n z}. \quad (15)$$

Substituting  $\psi_n^0(z)$  in the right part of equation

(14), we find the solution of the inhomogeneous equation.

$$\tilde{\psi}_n(z) = -\beta^2 q \tilde{\zeta}(N_{0d}) \times \left[ \frac{e^{i(k_{n-1} + ik_l)z}}{k_n^2 - (k_{n-1} + ik_l)^2} A_{n-1} - \frac{e^{i(k_{n+1} + ik_l)z}}{k_n^2 - (k_{n+1} + ik_l)^2} A_{n+1} \right]. \quad (16)$$

The solution of Schrodinger equation (11) we can represent as the series:

$$\psi_n(x, z, t) = \sum_{n=-\infty}^{\infty} \left[ A_n e^{ik_n z} - \frac{\beta^2 q \tilde{\zeta}(N_{0d}) e^{i(k_{n-1} + ik_l)z}}{k_n^2 - (k_{n-1} + ik_l)^2} A_{n-1} - \frac{\beta^2 q \tilde{\zeta}(N_{0d}) e^{i(k_{n+1} + ik_l)z}}{k_n^2 - (k_{n+1} + ik_l)^2} A_{n+1} \right] e^{i\Phi_n(x, t)}. \quad (17)$$

To find the dispersion law of surface electron states  $E = E(k_x)$ , we use the boundary conditions for the wave function at infinity and at the interface boundary. The wave function should be limited at  $x, z \rightarrow \infty$ , while on the surface  $z = z_0(x)$  boundary conditions can be of two types:

$$\psi|_{z=z_0(x)} = 0, \quad (18)$$

$$\bar{N} \bar{\nabla} \psi|_{z=z_0(x)} = 0, \quad (19)$$

where  $\bar{\nabla} = \bar{i} \frac{\partial}{\partial x} + \bar{k} \frac{\partial}{\partial z}$ ,  $\bar{N}$  is vector of normal to the surface with components

$$N_x = -\frac{\frac{\partial z_0}{\partial x}}{\left[ 1 + \left( \frac{\partial z_0}{\partial x} \right)^2 \right]^{1/2}}, \quad N_z = \frac{1}{\left[ 1 + \left( \frac{\partial z_0}{\partial x} \right)^2 \right]^{1/2}}. \quad (20)$$

For smooth roughness of the surface  $q\tilde{\zeta}(N_{0d}) \ll 1$  ( $\frac{\partial z_0}{\partial x} \ll 1$ ) the components of the normal vector are:

$$N_x = -\frac{\partial z_0}{\partial x}, \quad N_z = 1. \quad (21)$$

Taking into account the condition of smooth surface roughness, the boundary conditions (18), (19) on the plane  $z = 0$  will take the form:

$$\frac{\partial \psi}{\partial z} + \frac{\partial^2 \psi}{\partial z^2} z_0 - \frac{\partial \psi}{\partial x} \frac{\partial z_0}{\partial x} \Big|_{z=0} = 0 \quad (22)$$

### 3. DISPERSION EQUATIONS OF ELECTRON STATES ON THE SURFACE WITH ROUGHNESS CREATED BY ADSORBED ATOMS AND ACOUSTIC QUASI-RAYLEIGH WAVE

At distribution of surface acoustic wave the electrons on the surface are scattering on its deformation potential  $V(x, z, t)$  [11] within the volume, and also on the roughness, which are formed by both surface acoustic wave and heterogeneous distribution of adsorbed atoms. As a result, the harmonics are actuating with wave numbers  $k_{n+1}$  and  $k_{n-1}$ . Substituting in the boundary condition (22) the wave function (17), we obtain a recurrent formula which describes the relation between the amplitudes of the harmonics  $n-1$ ,  $n$ ,  $n+1$ :

$$\left\{ \begin{array}{l} \dots\dots\dots \\ L_{-1}A_{-1} + L_0A_0 + L_1A_1 = 0, \\ L_0A_0 + L_1A_1 + L_2A_2 = 0, \\ L_1A_1 + L_2A_2 + L_3A_3 = 0, \\ \dots\dots\dots \\ L_{n-1}A_{n-1} + L_nA_n + L_{n+1}A_{n+1} = 0, \\ \dots\dots\dots \end{array} \right. \quad (23)$$

where

$$L_{n\pm 1} = -\frac{\tilde{\zeta}(N_{od})}{2} \left[ k_{n\pm 1}^2 \mp q(k_x + (n \mp 1)q) \right] - \frac{i\beta^2 q \tilde{\zeta}(N_{od}) [k_{n\pm 1} + ik_l]}{k_n^2 - (k_{n\pm 1} + ik_l)^2},$$

$$L_n = ik_n + \frac{\beta^2 q \tilde{\zeta}^2(N_{od})}{2} \left[ \frac{(k_n + ik_l)^2 + q(k_x + (n+1)q)}{k_{n+1}^2 - (k_n + ik_l)^2} + \frac{(k_n + ik_l)^2 - q(k_x + (n-1)q)}{k_{n-1}^2 - (k_n + ik_l)^2} \right].$$

In the next calculations, the energy of the Rayleigh wave quantum is neglected, i.e.

$$\hbar\omega'(q, N_{od}) \ll \frac{\hbar^2 q^2}{2m^*} \quad \text{or} \quad \xi_0 c_t \ll \frac{\hbar q}{2m^*} \quad (24)$$

If the surface roughness are formed by a quasi-Rayleigh wave, then the electrons dissipate not only on the roughness created by the inhomogeneous distribution of adsorbed atoms  $N_d(x)$ , but also on the deformation potential of the quasi-Rayleigh wave. This additional scattering prevents the formation of surface electron states.

We will consider the possibility of the existence of surface electron states for zero harmonic  $A_0$  which interacts with harmonics  $A_{-1}$  and  $A_{+1}$ . In this case, the interaction with the harmonic  $n \geq 2$  is neglected, because the connection with the zero harmonic is proportional to  $(q\tilde{\zeta}(N_{od}))^n \ll 1$ . From the formula (23) we obtain a system of equations with respect to the amplitudes  $A_{-1}$ ,  $A_0$ ,  $A_{+1}$ . Equating to zero the determinant of the system (23), we find the spectrum of electron states on a surface with roughness, formed by the sur-

face acoustic wave and adsorbed atoms

$$k_0 = \frac{-\tilde{\zeta}^2(N_{od})}{4} \left[ \frac{(k_0^2 + k_x q)^2}{k_{-1}} + \frac{(k_0^2 - k_x q)^2}{k_1} \right] - \frac{i\beta^2 q \tilde{\zeta}^2(N_{od})}{2} \times$$

$$\times \left\{ \frac{k_0^2 + k_x q}{k_{-1}} \left[ \frac{k_0 + ik_l}{k_{-1}^2 - (k_0 + ik_l)^2} + \frac{k_{-1} + ik_l}{k_0^2 - (k_{-1} + ik_l)^2} \right] + \frac{k_0^2 - k_x q}{k_1} \times \right.$$

$$\times \left. \left[ \frac{k_0 + ik_l}{k_1^2 - (k_0 + ik_l)^2} + \frac{k_1 + ik_l}{k_0^2 - (k_1 + ik_l)^2} \right] - k_0 \left( \frac{\Gamma_1}{k_1} + \frac{\Gamma_{-1}}{k_{-1}} \right) + \Gamma_0 \right\}, \quad (25)$$

where

$$\Gamma_0 = \frac{q(k_x - q) - (k_0 + ik_l)^2}{k_{-1}^2 - (k_0 + ik_l)^2} - \frac{q(k_x + q) + (k_0 + ik_l)^2}{k_1^2 - (k_0 + ik_l)^2},$$

$$\Gamma_{\pm 1} = \frac{(k_{\pm 1} + ik_l) \mp k_x q}{k_0^2 - (k_{\pm 1} + ik_l)^2}.$$

The solution of equation (25)  $k_0$  we find by the method of successive approximations  $k_0(\tilde{\zeta}(N_{od})) = k_0(\tilde{\zeta}(0)) + \delta k_0(\tilde{\zeta}(N_{od}))$  for a small parameter  $q\tilde{\zeta} \ll 1$  regarding amplitudes  $A_{-1}$ ,  $A_0$ ,  $A_{+1}$ , where  $\tilde{\zeta}(N_{od}) = \tilde{\zeta}(0) + \delta\tilde{\zeta}(N_{od})$ ,  $\tilde{\zeta}(0)$  is the height of the roughness of the surface, created only by a surface acoustic wave.

For the case  $\tilde{\zeta}(N_{od}) = 0$  (the absence of the adsorbed atoms and a surface acoustic wave, i. e. the case of a smooth surface) the solution of equation (25) is  $k_0 \equiv k_0^{(0)} = 0$ . Then the dispersion law of electrons moving along a smooth surface has the form  $E_0 = \frac{\hbar^2 k_x^2}{2m^*}$ . In this case the region of electrons localization  $L_c(N_{od}) = \frac{1}{|\delta k_0(N_{od})|}$  occupies a half a space  $x \in (0; \infty)$ , since  $|\delta k_0(N_{od})| \rightarrow 0$ .

At  $n=0$   $k_0^2 = \frac{2m^*}{\hbar^2} E - k_x^2$ . Then

$$E = \frac{\hbar^2}{2m^*} (k_0^2 + k_x^2) = \frac{\hbar^2 k_x^2}{2m^*} \left( 1 + \frac{k_0^2}{k_x^2} \right). \quad (26)$$

Let  $k_0 = k_0^{(0)} + \delta k_0$ . Then

$$E = \frac{\hbar^2 k_x^2}{2m^*} \left( 1 + \frac{(\delta k_0)^2}{k_x^2} \right), \quad k_0^{(0)} = 0. \quad (27)$$

In the next approximation, for  $\tilde{\zeta} \neq 0$  the quantity  $\delta k_0$  is founded in the boundary cases: long-wave ( $k_x \ll q$ ), resonance ( $k_x = \frac{q}{2}$ ) and short-wave ( $k_x \gg q$ ) cases.

In the long-wave approximation the dispersion law of electron states has the form

$$E = \frac{\hbar^2 k_x^2}{2m^*} \left[ 1 + \frac{(k_x^2 - 2\beta^2)^2}{k_x^2} \frac{q^4}{16} \left( \frac{1}{k_1} + \frac{1}{k_{-1}} \right)^2 \tilde{\zeta}_0^3 (\tilde{\zeta}_0 + 4\delta\tilde{\zeta}(N_{od})) \right], \quad (28)$$

where  $k_1 = i\sqrt{q(q+2k_x)}$ ,  $k_{-1} = i\sqrt{q(q-2k_x)}$ .

In the resonance case the dispersion equation has the form

$$\delta k_0 \delta k_{-1} = -\frac{\tilde{\zeta}_0^2 + 2\tilde{\zeta}_0 \delta \tilde{\zeta}(N_{od})}{16} q^4 \left(1 - \frac{8\beta^2}{qk_l}\right),$$

where  $\delta k_0 = \sqrt{\frac{2m^*}{\hbar^2} \delta E - q \delta k_x}$ ;  $\delta k_{-1} = \sqrt{\frac{2m^*}{\hbar^2} \delta E + q \delta k_x}$ .

At the point  $k_x = \frac{q}{2}$  ( $k_x = \frac{\pi}{L_x}$ ) the energy changes

skippingly, i. e. there is a band gap which value is equal to

$$2\delta E = -\frac{\hbar^2 q^4}{16m^*} \left(1 - \frac{8\beta^2}{qk_l}\right) (\tilde{\zeta}_0^2 + 2\tilde{\zeta}_0 \delta \tilde{\zeta}(N_{od})) \quad (29)$$

As can be seen from formula (29), in the case of absence of adsorbed atoms ( $\delta \tilde{\zeta}(N_{od}) = 0$ ), the width of the band gap in the near-surface layer of the GaAs (100) semiconductor coincides with the results of work [7].

Figure 1 shows a plot of the dependence of the semiconductor band gap width on the concentration of adsorbed atoms on the plane GaAs(100) at the point of the Brillouin zone  $k_x = \frac{q}{2}$  or  $k_x = \frac{\pi}{L_x}$ . The upper and lower branches are determined accordingly to the relations:

$$E_+ \left(k_x = \frac{q}{2}\right) = -\frac{\hbar^2 q^2}{8m^*} \left[1 + \frac{q^2}{4} \left(1 - \frac{8\beta^2}{qk_l}\right) (\tilde{\zeta}_0^2 + 2\tilde{\zeta}_0 \delta \tilde{\zeta}(N_{od}))\right]; \quad (30)$$

$$E_- \left(k_x = \frac{q}{2}\right) = -\frac{\hbar^2 q^2}{8m^*} \left[1 - \frac{q^2}{4} \left(1 - \frac{8\beta^2}{qk_l}\right) (\tilde{\zeta}_0^2 + 2\tilde{\zeta}_0 \delta \tilde{\zeta}(N_{od}))\right]. \quad (31)$$

The calculation was made for a GaAs(100) semiconductor with the following parameter values [6]:

$$l_d = 2,9 \text{ nm}; \quad a = 0,565 \text{ nm}; \quad \lambda = 0,02 \text{ eV}; \quad T = 100 \text{ K};$$

$$c_l = 4400 \text{ m/s}; \quad c_t = 2475 \text{ m/s}; \quad \rho = 5320 \text{ kg/m}^3;$$

$$q = 0,03 \text{ \AA}^{-1}; \quad D_d = 5 \cdot 10^{-2} \text{ sm}^2/\text{s}; \quad \theta_d = 10 \text{ eV};$$

$$\frac{\partial F}{\partial N} = 0,1 \text{ eV}; \quad N_{od} = 3 \cdot 10^{13} \text{ sm}^{-2}; \quad m^* = 6,1 \cdot 10^{-32} \text{ kg}.$$

Figure 1 shows that the functional dependence of the band gap width on the concentration of adsorbed atoms is nonmonotonic. It is observed an increase of functional dependence  $\delta E = \delta E(N_{od})$  on the concentration interval of adatoms  $0 < N_{od} \leq 2,1 \cdot 10^{12} \text{ sm}^{-2}$ . At this concentration interval the semiconductor band gap width increases on 8%. With further increasing of the adsorbed atoms concentration, the band gap width decreases. Moreover, on the interval  $2,1 \cdot 10^{12} < N_{od} \leq 10^{13} \text{ sm}^{-2}$  the band gap width decreases on 56%. Such nonmonotonic dependence of  $\delta E = \delta E(N_{od})$  is explained by the nonmonotonic de-

portment of the dependence of the rough height  $\tilde{\zeta} = \tilde{\zeta}(N_{od})$  on the adsorbed atoms concentration [11].

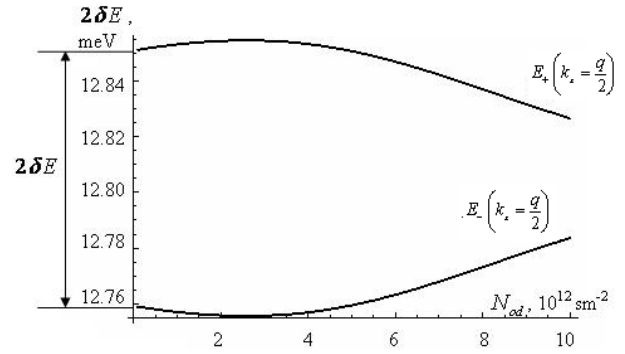


Fig. 1 – The band gap width on the surface of GaAs(100) semiconductor, depending on the concentration of adsorbed atoms

In the short-wave approximation the the values  $\delta k_0$  and  $E$  are complex, i. e. the electron states are quasi-stationary.

$$E = \text{Re } E + i \text{Im } E;$$

$$\text{Re } E = \frac{\hbar^2 k_x^2}{2m^*} \left[1 + \frac{(\text{Re } \delta k_0)^2 - (\text{Im } \delta k_0)^2}{k_x^2}\right];$$

$$\text{Im } E = \frac{\hbar^2}{2m^*} \text{Re } \delta k_0 \text{Im } \delta k_0 < 0,$$

where

$$\text{Re } \delta k_0 = -\frac{q^2}{k_{-1}} (\tilde{\zeta}_0^2 + 2\tilde{\zeta}_0 \delta \tilde{\zeta}(N_{od})) (k_x^2 + 2\beta^2);$$

$$\text{Im } \delta k_0 = -\frac{q^2}{4|k_l|} (\tilde{\zeta}_0^2 + 2\tilde{\zeta}_0 \delta \tilde{\zeta}(N_{od})) (k_x^2 - 2\beta^2);$$

$$k_1 = i\sqrt{q(q+2k_x)}; \quad k_{-1} = \sqrt{q(2k_x - q)}.$$

At the same time the relaxation time is  $\tau = \hbar / |\text{Im } E|$ .

The length of the spatial localization of electron wave function  $L_e = L_e(N_{od})$  in the long-wave approximation we obtain by the relation:

$$L_e(N_{od}) = \frac{4}{q^2 \left(\frac{1}{k_1} + \frac{1}{k_{-1}}\right) (\tilde{\zeta}_0^2 + 2\tilde{\zeta}_0 \delta \tilde{\zeta}(N_{od})) (k_x^2 - 2\beta^2)}. \quad (32)$$

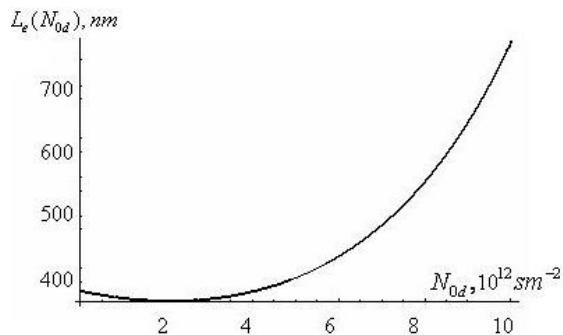
From formula (32) we can see, that the reduction of roughness period  $L_x$  ( $q = \frac{2\pi}{L_x}$ ) along the  $x$  axis or the increasing of the height  $\tilde{\zeta}(N_{od}) = \tilde{\zeta}_0 + \delta \tilde{\zeta}(N_{od})$  of the adsorbed surface roughness leads to a stronger localization of electron wave function

$$\psi_0 = A_0 e^{ik_x x - z/L(N_{od})}$$

The decrease of the length of the electron de Broglie wave reduces to the same effect (increase of  $k_x$ ).

Figure 2 shows the dependence of the length of the

spatial localization of electron wave function  $L_e = L_e(N_{od})$  on the adsorbed atoms concentration in the case of long-wave approximation.



**Fig. 2** – The length of the spatial localization of electron wave function in the subsurface of GaAs (100) semiconductor, depending on the concentration of adsorbed atoms at  $k_x = q/3$ ;  $q = 0.03 \text{ 1/\AA}$

Analyzing the graphical dependence on figure 2, we see that curve  $L_e = L_e(N_{od})$  is nonmonotonous. At small concentrations of adsorbed atoms ( $0 < N_{od} \leq 2,1 \cdot 10^{12} sm^{-2}$ ) with increasing concentration the length of the spatial localization of the wave function of the electron decreases. With a further increase of adsorbed atoms concentration, the function

$L_e = L_e(N_{od})$  is increasing monotonously.

#### 4. CONCLUSIONS

The spectrum of surface electron states on the adsorbed solid surface was obtained under the action of a surface acoustic wave, within the approximation of the interaction of the first three electron harmonics ( $n = -1, 0, +1$ ) in the long-wave ( $k_x \ll q$ ), resonance ( $k_x = \frac{q}{2}$ ) and short-wave ( $k_x \gg q$ ) cases.

It was shown that there are two regions in the spectrum of surface electron states, which are separated by a band gap, whose value changes depending on the concentration of adsorbed atoms.

It has been established that the dependence of band gap width on the semiconductor surface, at the edge of the first Brillouin zone, on the concentration of adsorbed atoms has the nonmonotonic character. At small concentrations of adatoms, the width increases when the concentration increases, while the length of the spatial localization of the electron wave function decreases. At higher concentrations  $2,1 \cdot 10^{12} < N_{od} \leq 10^{13} sm^{-2}$  the energy width narrows when the concentration increases. In this case, the length of the spatial localization increases.

### Електронні стани на нерівній поверхні GaAs (100), створеній поверхневою акустичною хвилею та адсорбованими атомами

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Розвинуто теорію електронних станів на поверхні напівпровідника з нерівностями, які створені як адсорбованими атомами, так і акустичною квазірелеєвською хвилею. Отримано спектр поверхневих електронних станів на адсорбованій поверхні напівпровідника GaAs у довгохвильовому, резонансному та короткохвильовому наближеннях з урахуванням взаємодії перших трьох електронних гармонік при дії акустичної квазірелеєвської хвилі. Показано, що залежності енергетичної ширини забороненої зони на поверхні напівпровідника і довжини просторової локалізації хвильової функції електрона від концентрації адсорбованих атомів в інтервалі  $0 < N_{od} \leq 10^{13} sm^{-2}$  мають немонотонний характер.

**Ключові слова:** Адсорбовані атоми, Акустична квазірелеєвська хвиля, Електронні стани.

### Электронные состояния на неровной поверхности GaAs (100), созданной поверхностной акустической волной и адсорбированными атомами

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Развита теория электронных состояний на поверхности полупроводника с неровностями, которые созданы как адсорбированными атомами, так и акустической квазірелеєвської волной. Получено спектр поверхностных электронных состояний на адсорбированной поверхности полупроводника GaAs в длинноволновом, резонансном и коротковолновом приближениях с учетом взаимодействия первых трёх электронных гармоник при воздействии акустической квазірелеєвської волны. Показано, что зависимости энергетической ширины запрещенной зоны на поверхности полупроводника и длины пространственной локализации волновой функции электрона от концентрации адсорбированных атомов в интервале  $0 < N_{od} \leq 10^{13} sm^{-2}$  имеют немонотонный характер.

**Ключевые слова:** Адсорбированные атомы, Акустическая квазірелеєвська волна, Электронные состояния.

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