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JOINT INFLUENCE OF INTERNAL FIELDS AND INDIUM SURFACE SEGREGATION ON BAND STRUCTURE IN INGAN/GAN SINGLE QUANTUM WELL

In this paper, authors investigate the influence of the indium surface segregation and piezoelectric polarization on the band structure of the InGaN/GaN single quantum well. The obtained results evidence that the indium surface segregation leads to the blue shift of the transition energy (70 meV for the segregation length 1nm at both heterointerfaces) while the piezoelectric polarization itself causes the read shift. Joint action of both effects influence on the potential profile determining the linear dependence of the transition energy on the width of the quantum well. The piezoelectric polarization is prevailed for the high indium amount, and the indium surface segregation is dominated for the low indium amount in the In(x)Ga(1-x)N alloy.

INTRODUCTION

Light-emitting diodes and semiconductor lasers based on InGaN/GaN quantum well structure are of actual interest due to their operation in the spectral range from the visible to the UV radiation [1]. On the other hand, a widespread application and designing of these devices is limited by existed difficulties concerning predictions of their optical spectral characteristics. Indeed, all published theories of the optical response of considered structures contain at least one fitting parameter. The most frequently encountered one is the linewidth of the inhomogeneous broadening [1], [2]. This kind of the broadening is related to 3D random variations of the potential relief caused by the indium composition fluctuations. Effects changing uniform indium distribution are the indium surface segregation [3], [4] and clustering [5]. In this letter, we focus on the indium surface segregation (ISS) and its influence on the band structure in InGaN/GaN single quantum well structure. The aim of this work is the theoretical investigation of traits in the band structure which are caused by the ISS and piezoelectric effects.

As a rule, the ISS is investigated experimentally by using the transition electron microscopy (TEM) [6], [7], reflection high energy electron diffraction (RHEED) [8] and X-rays diffraction (XRD) [9]. All these methods have own disadvantages in case of ultrathin quantum wells. TEM could induce an additional local strain in the crystal lattice after a long duration of the electron beam exposition time [10]. RHEED is realized during the crystal growth and cannot be applied after the fabrication. The XRD technique has low sensitivity for distances up to 2 nm and its experimental data are difficult to interpret. The optical spectroscopy avoids most of these disadvantages. However, the application of the optical spectroscopy requires the theory providing clear connection between the optical spectroscopic data and parameters of the structure imperfections.

Knowing of the band structure is necessary for computations of the optical characteristics using Fermi's Golden Rule, density matrix approach or Green's function method. That is caused the topicality of this paper.

INDIUM DISTRIBUTION PROFILE

There are several approaches to modeling and parametrization of the indium profile in the structure with segregation. One of them is based on the Fick's law [6]. This approach gives the indium distribution profile expressed as a linear combination of the complementary error functions:

$$n_{In}(z)=\frac{n_{nom}}{2}\left[erfc\left(\frac{w_{nom}-2z}{2L_1}\right)+erfc\left(\frac{w_{nom}+2z}{2L_2}\right)\right] \quad (1)$$

here: $n_{In}(z)$ is the indium distribution, n_{nom} is the nominal indium molar fraction in QW layer, w_{nom} is the nominal width of QW, L_1 and L_2 are lendth of the surface segregation.

Some authors use the Gaussian function for potential profile approximation for QWs where surface segregation effects take place. In this case, the width of the Gaussian function is a fitting parameter which can be found from experimental data or theory treatment. Gaussian approximation gives symmetrical indium distribution function. However, TEM images of QW structures argue that the surface segregation leads to asymmetrical shape of the indium distribution profile. Therefore, we use more complicated description of the surface segregation based on kinetic equations [7]. The solution of the coupled kinetic equations is fitted by the following expression [3]:

$$n_{In}(z)=\begin{cases} 0, & z \le z_1, \\ n_0 erf\left(\frac{z-z_1}{L_1}\right), & z_1 < z \le z_2, \\ n_0 erf\left(\frac{z_2-z_1}{L_1}\right)\left[1-n_0 erf\left(\frac{z-z_1}{L_1}\right)\right], & z_2 \le z. \end{cases} \quad (2)$$

here $z_2 - z_1 = w_{nom}$

This formula approximates with high accuracy the indium distribution obtained by means of the theory of Muraki *et al.* [11], [12]. Expression (2) gives asymmetrical indium distribution. This approximation contains two fitting parameters instead of single one as in case of Gaussian approximation. That gives more freedom to provide accurate fitting. As it follows from the experimental data, fitting parameters L_1 and L_2 are not equal that means inequality of the segregation effect for switch-on and switch-off regimes of the MBE indium source evaporator. Hereafter, we name parameters L_1 and L_2 the segregation lengths.

POSITION-DEPENDENT MATERIAL PARAMETERS AND INTERNAL ELECTRIC FIELDS

In this paper, we consider nitride single quantum well structure with layers made of In(x)Ga(1-x)N and GaN semiconductor alloys. All position-dependent material parameters except the band gap energy have been computed using linear interpolation formulas. We use the second order interpolation formula with the bowing parameter to compute the band gaps. Material parameters for relevant binary semiconductors have been taken from [17]. In the case of In(x)Ga(1-x)N QW heterostructure, the molar fraction of indium x is a position-dependent parameter. All other position-depended quantities are related to the indium distribution in the structure.

Well-known peculiarity of the wurtzite crystal heterostructure is strong internal electric fields caused by spontaneous polarization and piezoelectric effects. In this paper, we neglect the spontaneous polarization and focus our attention on piezoelectric fields. This is good approximation in case of high indium amount in In(x)Ga(1-x)N alloy.

High indium amount leads to significant lattice constant mismatch for In(x)Ga(1-x)N/GaN material pair. Lattice mismatch causes strong strain giving origin to piezoelectric effects. Piezoelectric polarization P_{piezo} is calculated using Vegard's interpolation formula [13]:

$$P_{piezo}(z) = xP^{InN}_{piezo}[\varepsilon(z)] + (1 - x)P^{GaN}_{piezo}[\varepsilon(z)] \quad (3)$$

where the strain coefficient $\varepsilon(z)$ is defined as

$$\varepsilon(z) = \frac{a_{subs} - a(z)}{a(z)} \quad (4)$$

here a_{subs} is the lattice constant of the substrate and $a(z)$ is the lattice constant of the unstrained semiconductor alloy at a point z.

As has been shown in Ref. [13], piezoelectric polarization of binary strained semiconductors can be expressed as:

$$P^{InN}_{piezo}(\varepsilon(z)) = -1.373\varepsilon(z) + 7.559\varepsilon^2(z) \quad (5)$$

$$P^{GaN}_{piezo}(\varepsilon(z)) = -0.918\varepsilon(z) + 9.541\varepsilon^2(z) \quad (6)$$

When the piezoelectric is absent, the quantum well is characterized by the square potential profile. The piezoelectric effect leads to zigzag shape of the quantum well.

BAND STRUCTURE

The electron wave function is obtained as solution of the Ben-Daniel-Duke equation resulted from joint action of the single-band and the envelope function approximations [16]. This approach is based on the following representation of the electron wave function [15]:

$$\left\langle r \middle| \psi^e_j \right\rangle = \exp\left(i\vec{k}_{\|}\vec{r}_{\|}\right)\phi_j(z)\left\langle r \middle| S \right\rangle, \quad (7)$$

where $\left\langle r \middle| S \right\rangle$ is the periodic Bloch function in the position-coordinate representation, $\phi_j(z)$ is the envelope function for the electron's j-th state, $\vec{k}_{\|}$ is in-plane wave vector and $\vec{r}_{\|}$ is the in-plane radius-vector. Solving of the Ben-Daniel-Duke problem gives unknown envelope functions $\phi_j(z)$ and band structure of the conduction band. The valence band structure is computed separately in more complicated manner to include into consideration intense band mixing effects. In the frame of the envelope function approximation, we use six-band model including into consideration interaction between heavy hole, light hole and spin-orbit split-off states with all possible directions of the spin. This approximation is widely used for semiconductor nitrides with wurtzite crystal structure [14]. In this case, wave functions for the valence band are represented as [13]:

$$\left\langle r \middle| \psi^h_j \right\rangle = \exp\left(i\vec{k}_{\|}\vec{r}_{\|}\right) \sum_{\substack{m=X\uparrow,Y\uparrow \\ Z\uparrow,X\downarrow,Y\downarrow,Z\downarrow}} \sum_{j=1}^{N_m} g^m_j(z)\left\langle r \middle| m \right\rangle, \quad (8)$$

where m m is an index indicating type of the basis function in the bulk Hamiltonian, N_m is number of considered subbands for the m-th band, $\left\langle r \middle| m \right\rangle$ is the periodic Bloch function of the m-th type and g^m_j are the

hole envelope functions.

Usually, to simplify the problem, the block-diagonal representation of Hamiltonian is applied. In this case, the problem is solved for each block of the Hamiltonian separately. The wave functions in the block-diagonal representation are modified as:

$$\left\langle r \middle| \psi_j^h \right\rangle = \exp\left(i\vec{k}_\parallel \vec{r}_\parallel\right) \sum_{\sigma=U,L} \sum_{m=1}^{3} \sum_{j=1}^{N_m} g_{j,\sigma}^m(z) \langle r | m \rangle, \quad (9)$$

here index σ refers to upper $\sigma = U$ or lower $\sigma = L$ blocks of the Hamiltonian. The 6×6 Hamiltonian in block-diagonal form [14] is

$$H_{6\times6} = \begin{pmatrix} H^U & 0 \\ 0 & H^L \end{pmatrix}, \quad (10)$$

with H^U and H^L being

$$H^U = \begin{pmatrix} F & K & -iH \\ K & G & \Delta - iH \\ iH & \Delta + iH & \lambda \end{pmatrix}, \quad (11)$$

$$H^L = \begin{pmatrix} F & K & iH \\ K & G & \Delta + iH \\ -iH & \Delta - iH & \lambda \end{pmatrix}, \quad (12)$$

here: $F = \Delta_1 + \Delta_2 + \lambda + \theta$, $G = \Delta_1 - \Delta_2 + \lambda + \theta$,

$$\lambda = \frac{\hbar^2}{2m_0}\left(A_1 k_z^2 + A_2 k_t^2\right) + \lambda_\varepsilon,\ \lambda_\varepsilon = D_1\varepsilon_{zz} + D_2\left(\varepsilon_{xx} + \varepsilon_{yy}\right),$$

$$\theta = \frac{\hbar^2}{2m_0}\left(A_3 k_z^2 + A_4 k_t^2\right) + \theta_\varepsilon,\ \theta_\varepsilon = D_3\varepsilon_{zz} + D_4\left(\varepsilon_{xx} + \varepsilon_{yy}\right),$$

$$\varepsilon_{xx} = \varepsilon_{yy} = \frac{a_{subs} - a}{a},\ \varepsilon_{zz} = -\frac{2C_{13}}{C_{33}}\varepsilon_{xx}, \varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{zx} = 0,$$

$$K = \frac{\hbar^2}{2m_0} A_5 k_t^2,\ H = \frac{\hbar^2}{2m_0} A_6 k_t k_z,\ \Delta = \sqrt{2}\Delta_3,$$

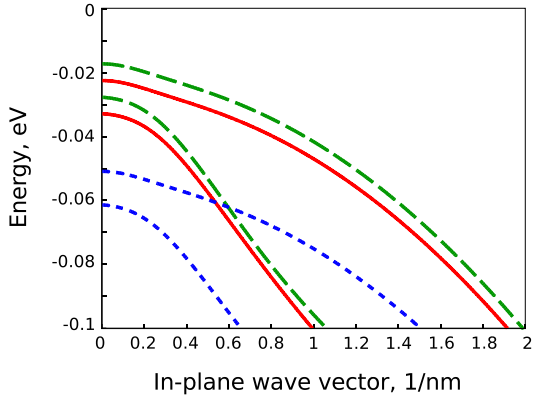
$k_t = \left|\vec{k}_\parallel\right|$, A_j ($j = 1 \div 5$) are valence-band structure parameters, D_j ($j = 1 \div 4$) are deformation potentials, Δ_1, Δ_2, Δ_3 are energy parameters, C_{13} and C_{33} are elastic stiffness constants.

In the frame of the envelope function approximation, Hamiltonian (10) is transformed to the differential operator using the transformation $k_z \to \partial/\partial z$. The band structure and envelope functions have been computed numerically, applying the finite difference method [14].

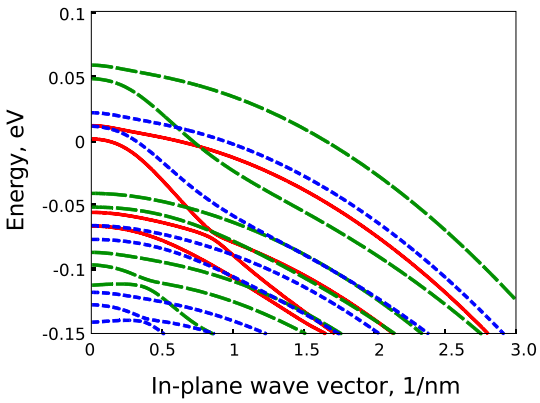
BAND STRUCTURE

We restrict our consideration here only by the valence band due to its more complicated structure comparing with conduction band.

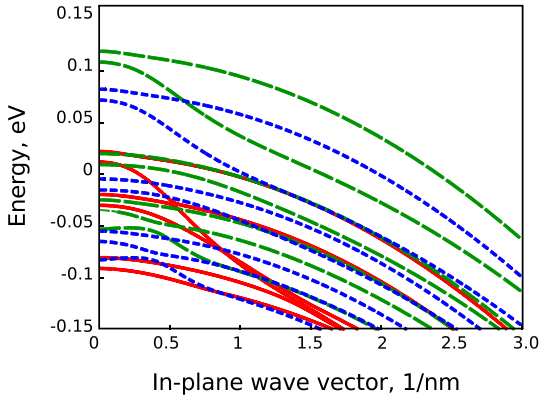
Computed band structures presented in Fig. 1 uncover effects of joint action of the piezoelectric polarization and indium surface segregation for semiconductor heterostructures with different indium amount (with different depths of the quantum well). Here, the indium surface segregation lengths equals $L_1 = L_2 = 1$ nm that corresponds to the experimental data [2]. As it follows from Fig.1, indium surface segregation does not lead to changes in the shape of the valence band dispersion curves. It means that the influence of surface segregation on the effective mass of carriers is not significant. Also, one can observe the blue energy shift of all states caused by the indium surface segregation effect. The energy shift is equal 20 meV for the conduction band and 50 meV for the valence band. Total blue shift is 70 meV.



a)



b)



c)

Fig. 1 – Band structures for InGaN/GaN single quantum well with indium amount a) x=0.1, b) x=0.2 and c) x=0.3 for square quantum well (solid curve), quantum well with piezoelectric polarization (dashed curve) and joint action of piezoelectric polarization and indium surface segregation (dotted curve)

For all considered cases, the piezoelectric polarization leads to significant shift of energy subbands in both conduction and valence bands. The resulted shift of the transition energies is red one for all cases that is opposite to the ISS. This feature of the nitrite quantum well structures is well-known and it is proved by several experimental works. Increasing of the indium amount leads to increasing of such an energy shift. That is caused by direct relation between indium amount and piezoelectric polarization following from Eq. 3.

As follow from presented results, the indium surface segregation leads to constant energy shift of subbands relative to subbands for the case when the piezoelectric polarization is present. In the shallow quantum well, the piezoelectric polarization in weak and the indium surface segregation is dominant causing strong blue shift. In the case when the indium amount is equal, the piezoelectric polarization and indium surface segregation have almost the same effect. Acting in opposite direction, their joint action does not change the energy of subbands significantly relative to their position in the square quantum well. At high indium amounts, the indium surface segregation just compensates the piezoelectric effect a little bit.

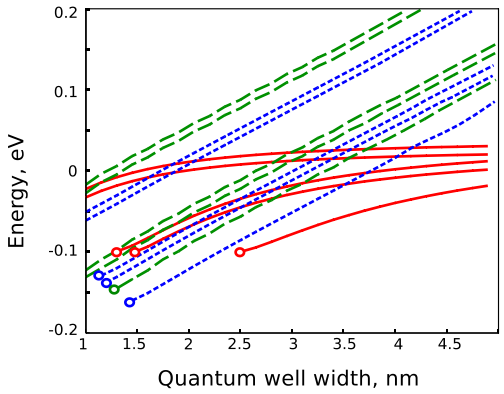
WIDTH DEPENDENCE OF THE BAND STRUCTURE

Fig. 2 contains dependences of the valence band edges on the quantum well width. In the case of the square quantum well, dependences of the band edges on the width of the quantum well are nonlinear ones. Especially, this is well-observed for holes which have lager effective mass. The piezoelectric polarization leads to zigzag potential profile of conduction and valence band edges. As s result, the dependence of the band edges on the quantum well width becomes linear. The ISS does not change the charter of this dependence significantly leading to some constant energy shift of subbands. This is the case for both conduction and valence bands.

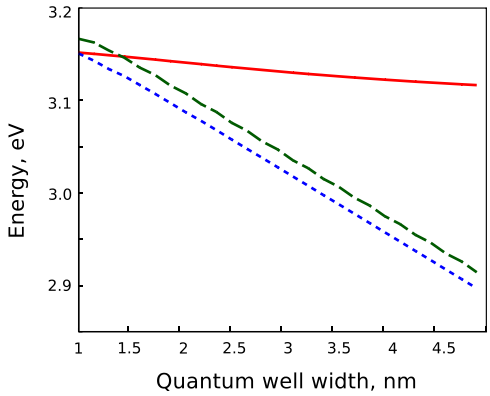
Changes in the width of the quantum well can lead to appearing of new confinement states in the quantum well. Such states are denoted by circles in Fig. 2. Conduction band have only one confined state in all cases.

CONCLUSIONS

In this paper, we have investigated the influence of the piezoelectric polarization and indium surface segregation on the band structure in InGaN/GaN single quantum well. Obtained results evidence that the joint action of the piezoelectric polarization and indium surface segregation cause unique position of subbands at the energy axis. The low indium amounts, the indium surface segregation is dominant effect due to piezoelectric polarization is weak in this case. However, the piezoelectric effects are prevailed at the high indium amount. Joint action of the indium surface segregation and piezoelectric polarization causes linear dependence of band edges on the width of the quantum well. This result is confirmed by experimental data based on the photoluminescence measurements [19].



a)



b)

Fig. 2 – Dependences of a) valence and b) conduction band edges on the quantum well width for the square quantum well (solid line), quantum well with piezoelectric fields (dashed line) and

quantum well with joint action of piezoelectric polarization and indium surface segregation (dotted line)

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In this paper, authors investigate the influence of the indium surface segregation and piezoelectric polarization on the band structure of the InGaN/GaN single quantum well. The obtained results evidence that the indium surface segregation leads to the blue shift of the transition energy (70 meV for the segregation length 1nm at both heterointerfaces) while the piezoelectric polarization itself causes the read shift. Joint action of both effects influence on the potential profile determining the linear dependence of the transition energy on the width of the quantum well. The piezoelectric polarization is prevailed for the high indium amount, and the indium surface segregation is dominated for the low indium amount in the In(x)Ga(1-x)N alloy.
Key words: surface segregation, internal fields, structure.

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СОВМЕСТНОЕ ВЛИЯНИЕ ВНУТРЕННИХ ЕЛЕКТРОСТАТИЧЕСКИХ ПОЛЕЙ И ПОВЕРХНОСТНОЙ СЕГРЕГАЦИИ ИНДИЯ НА ЗОННУЮ СТРУКТУРУ В INGAN/GAN ОДИНОЧНОЙ КВАНТОВОЙ ЯМЕ

В этой работе, авторы исследуют влияние поверхностной сегрегации индия и пьезоэлектрической поляризации на зонную структуру InGaN/GaN одиночной квантовой ямы. Полученные результаты свидетельствуют, что поверхностная сегрегация индия приводит к «синему» сдвигу энергии перехода (70 мэВ для длины сегрегации 1 нм на каждом гетероинтерфейсе) в то время как пьезоэлектрическая поляризация обуславливает «красный» сдвиг. Совместное действие обоих эффектов оказывает влияние на потенциальный профиль определяя линейную зависимость энергии перехода от ширины квантовой ямы. Пьезоэлектрическая поляризация является преобладающей при больших содержаниях индия, а поверхностная сегрегация индия преобладает при малом содержании индия в In(x)Ga(1-x)N твердом растворе.

Ключевые слова: поверхностная сегрегация, структура, квантовое поле.

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СУМІСНИЙ ВПЛИВ ВНУТРІШНІХ ЕЛЕКТРОСТАТИЧНИХ ПОЛІВ ТА ПОВЕРХНЕВОЇ СЕГРЕГАЦІЇ ІНДІЯ НА ЗОННУ СТРУКТУРУ В INGAN/GAN ПООДИНОКІЙ КВАНТОВІЙ ЯМІ

У роботі автори досліджують вплив поверхневої сегрегації індія і п'єзоелектричної поляризації на зонну структуру InGaN/GaN поодинокої квантової ями. Отримані результати свідчать, що поверхнева сегрегація індія приводить до «синього» зміщення енергії переходу (70 мэв для довжини сегрегації 1 нм на кожному гетероінтерфейсі) у той час як п'єзоелектрична поляризація обумовлює «червоне» зміщення. Спільна дія обох ефектів впливає на потенційний профіль визначаючи лінійну залежність енергії переходу від ширини квантової ями. П'єзоелектрична поляризація є переважаючою при великому вмісті індія, а поверхнева сегрегація індія переважає при малому вмісті індія в In(x)Ga(1-x)N твердому розчині.

Ключові слова: поверхнева сегрегація, структура, квантове поле.