OPTO-ELECTRONICS REVIEW **12**(4), 441–443

Exciton energies and probability of their radiative decay in GaN/AlN quantum structures

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Exciton energies and probabilities of radiative transition from exciton state are calculated in GaN/AlN quantum dots. Electric field conditioned by strain induced and spontaneous polarization is considered by means of tight bind approximation, electron-hole Coulomb interaction is calculated by means of perturbation theory. Despite the presence of an electrical field, the calculated Coulomb energy is significantly increased with respect to bulk material. In large dots, the Coulomb term as well as probability of radiation transition for higher energetic excitons was strongly increased.

Keywords: GaN, quantum dots, excitons.

1. Introduction

Semiconductor quantum dots (QDs) are of interest both from fundamental and practical points of view because they on the one hand enable us to study zero-dimensional objects, so-called artificant atoms, and on the other hand have attractive perspectives for device application. Recent years QD structures of high quality have been successfully grown and investigated using wide range of semiconductor compounds: GaAs based III–V QDs [1–3], ZnSe based II–VI QDs [4–6] as well as InP, GaSb, PbS based IV–VI, and nitride structures [7–9]. Among these structures nitride-based quantum dots take special place, which is conditioned by the fact that wurtzite III–nitrides, because of noncentrosymmetry, exhibit large effect of spontaneous and strain induced polarization. The piezoelectric coefficients are almost an order of magnitude larger than in other III–V compounds. Large amount of polarization charge appears at the heterointerface even in the absence of strain due to the difference in the spontaneous polarization across the interface. The very strong internal electric field induced by the polarization charge has a dramatic effect on the properties of nitride QDs.

In this paper, we studied the influence of the built-in electrostatic field on the energies of excitons and probabilities of their radiative decay. Energy levels of electrons and holes are calculated using a single-particle model in a single band effective mass approximation. Electrostatic potential is considered in a tight bind approximation. Electron-hole Coulomb interaction is accounted in the framework of perturbation theory.

2. Calculations and results

The effects of quantum confinement strain and polarization including strain induced and spontaneous polarization determine the energies of excitons in quantum dots.

GaN QDs are fully strained in the AlN matrix and exhibit almost no interdiffusion [9], so the model of a particle in a rectangular potential well with finite barriers satisfactorily describes the confinement potential. At the GaN/AlN interface, the barrier height is 2.1 eV for electrons and 0.7 eV for holes.

For GaN QDs grown on AlN, the strain is commonly compressive which induces a blue shift in the band gap. This shift is proportional to the strain. In the case of vanishing shear strain for fully strained GaN on AlN ~0.25 eV blue shift of band gap is obtained [10]. This value is taken into account when calculating exciton energies.

In contrast to the effects of confinement and strain, the polarization effect induces a red shift of exciton energies. Both spontaneous polarization and strain induced polarization (piezoelectric effect) produce large electric field. Electric field has arisen because of spontaneous polarization is proportional to the difference of spontaneous polarization at the GaN/AlN interface; additional polarization induced by strain can be calculated from the elastic and piezoelectric constants: $P_z = 2e_{31}\varepsilon_{xx} + e_{33}\varepsilon_{zz}$. Experimental and theoretical estimations define total electric field between 3.8–5.5 MV/cm [9,11,12]. This huge field drives electrons in the GaN towards the top interface and holes towards the bottom interface. As a result, the electron-hole transition energy is strongly reduced and their recombination probability decreases. In the following calculations, the lowest value of built-in electrical field is taken.

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The self-assembled GaN QDs have a disk-like shape with a base diameter a few times larger than height; the diameter was observed to depend approximately linearly on a dot height [8]. Therefore lateral effects of confinement must be less pronounced than vertical conferment effect. That is why we consider only z coordinate dependent problem.

First, non-interacting particles are considered in the potential well asimmetrized by an electrical field (Fig. 1) corresponding inside the dots to the following Schrödinger equation

$$\frac{d^2\Psi(Z_{e(h)})}{dz_{e(h)}^2}+\frac{2m_{e(h)}^*}{\hbar^2}\left(E-U_0^{e(h)}-eE_{elc}z_{e(h)}\right)=0, \quad (1)$$

where $m_{e(h)}^*$ are the electron (hole) effective masses, $U_0^{e(h)}$ is the potential barrier for electrons (holes) equal to ~75% conductive (valence) band offsets at the GaN/AlN interface, and E_{elc} is the electrostatic field. Outside the dots an electric field is assumed to have the same absolute value as inside the dots.

To solve the problem of motion of particles in such a potential, their wave functions are presented as a sum of eigenfunctions of a particle in the rectangular well with a finite potential barrier

$$\Psi_i^{e(h)}(z_{e(h)})=\sum_{k=1}^{n(m)}C_{ik}^{e(h)}\varphi_k^{e(h)}(z_{e(h)}), \quad (2)$$

where $\varphi_k^{e(h)}$ are the eigenfunctions of electrons (holes) in rectangular well with finite barrier [12], n and m are the numbers of bound states of electrons and holes in a rectangular well.

The eigenvalues $E_i^{e(h)}$ and the corresponding set $C_{ik}^{e(h)}$ of coefficients are found by matrix diagonalization method.

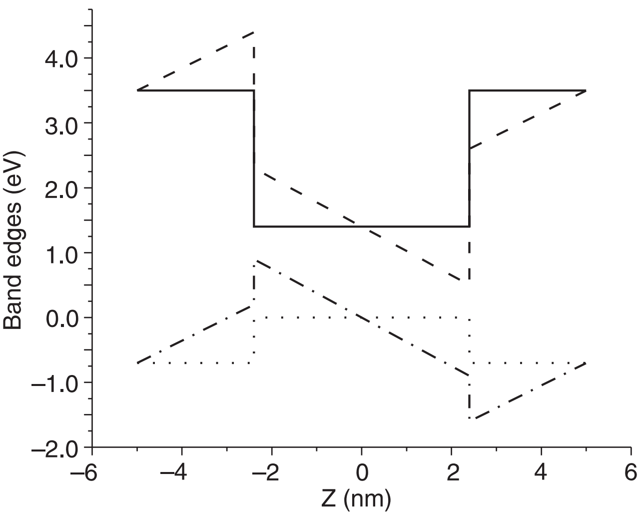

Fig. 1. Variation of conduction and valence band edges in GaN/AlN quantum dots along the growth direction. Band-edge profiles without electrostatic field is also presented.

Electron-hole Coulomb interaction is accounted by means of perturbation theory. The Coulomb correction to a state with electrons and holes in i and j state respectively are given in terms of single particle wave functions expressed by Eq. (2)

$$J_{i,j}=\int\frac{\left|\Psi_i^e(z_e)\right|^2\left|\Psi_j^h(z_h)\right|^2}{\varepsilon\sqrt{\rho^2+(z_e-z_h)^2}}dz_e dz_h, \quad (3)$$

where ε is the dielectrical constant of the quantum dot, and ρ is in-plane electron-hole distance. As lateral confinement is neglected it is taken equal to that of bulk material. Finally, the energies of excitons are calculated by the formula

$$E_{i,j}=E_i^e+E_j^h+E_g+E_{str}-J_{i,k}, \quad (4)$$

where E_i^e and E_j^h are accounted from the bottom of conductive and top of valence, band for bulk GaN, respectively, E_g is the band gap, and E_{str} is the strain induced blue shift.

Existence of electrostatic field should strongly influence probability of radiation decay of excitons. The probability P of radiative transition from the exciton state described by the wave function $\Phi(z_e,z_h)$ is proportional to the integral

$$P\sim\left|\int dz_e dz_h\Phi(z_e,z_h)\delta(z_e-z_h)\right|^2. \quad (5)$$

The calculations showed that ground state wave functions of electrons and holes are significantly shifted to the opposite edges of QDs. Consequently, the probability of radiative transition is close to zero. The probability of radiation decay significantly increases for higher energetic excitons, because wave functions of electrons and holes of higher levels are shifted to the area of higher potential that is, to the centre of dots, which increases their overlapping.

In Fig. 2(a), the probability of radiative transition versus exciton energy is presented for 4.8 nm dot vertical size. The exciton energies are between 2.8 eV and 6.5 eV. The highest exciton "density" is in 4–5 eV energy range. In the same area, the probability of radiative decay has the maximum value. Electron-hole Coulomb attraction energy exhibits the same behaviour, it ranges between 40–68 meV and has the maximum in the same energy range. The picture is less pronounced for smaller QDs (2.4 nm height) where polarization effects are not so significant as in large QDs [Fig. 2(b)]. For smaller QDs, the probabilities of radiative transition of ground state excitons are not very low and Coulomb interaction is almost the same (~65 meV) for ground state and excited state excitons. As it can be seen, despite the presence of electrical field, the exciton binding energy in GaN QDs significantly exceeds that for bulk material indicating strong carrier confinement. This in its turn

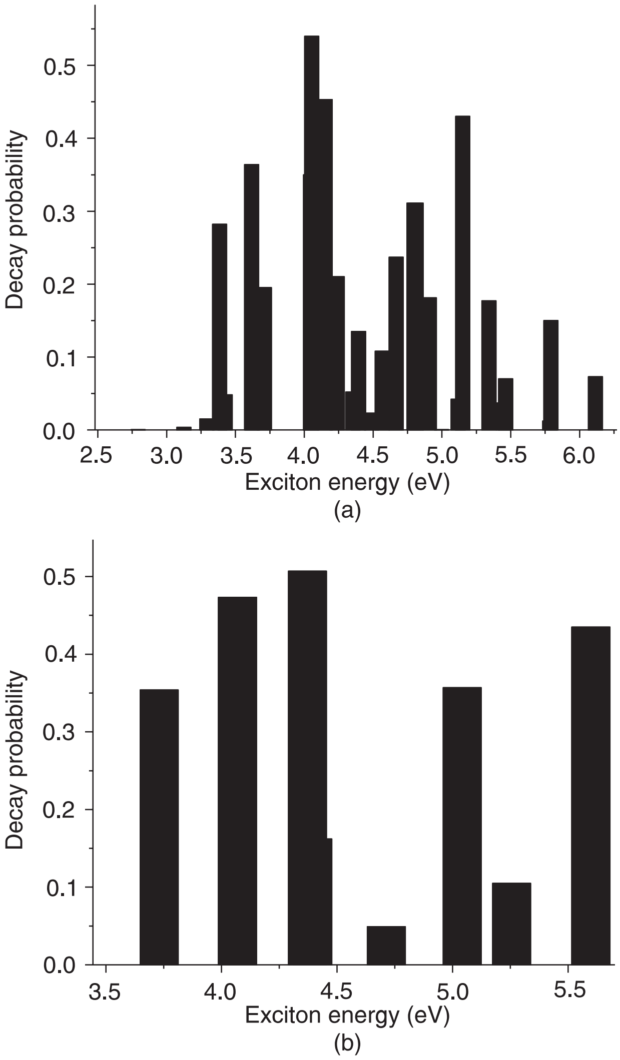

Fig. 2. Probability of radiation transition of excitons versus energy: dot height is 4.8 nm (a) and dot height 2.4 nm (b).

is conditioned by high potential barrier for electrons and large effective mass of holes.

Acknowledgements

This work is supported by grant (FEL. RIG 980760) of NATO Science Program.

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