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Microelectronics Journal 38 (2007) 663–666

Microelectronics Journal

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Hydrogenic impurity in zinc-blende GaN/AlGaN quantum dot

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Received 14 April 2007; accepted 3 June 2007
Available online 23 July 2007

Abstract

Within the framework of effective-mass approximation, we have calculated the binding energy of a hydrogenic donor impurity in a zinc-blende (ZB) GaN/AlGaN cylindrical quantum dot (QD) using a variational procedure. It is found that the donor binding energy is highly dependent on the impurity position and QD size. The donor binding energy E_b is largest when the impurity is located at the center of the QD. The donor binding energy is decreased when the QD height (radius) is increased.

PACS: 73.21.La; 71.55.−i

Keywords: Quantum dot; Hydrogenic impurity; Donor binding energy

1. Introduction

The progress in the growth and electronic quality of group-III nitrides has been very rapid in the last few years, as illustrated by the realization of bright blue and green light emitting diodes and near-UV laser diodes [1,2]. Group III-nitrides can be produced in the thermodynamic stable configuration with wurtzite (WZ) crystal structure and in the metastable modification with zinc-blende (ZB) structure [3]. The existence of the built-in electric field in the WZ GaN/AlGaN quantum well due to the spontaneous and piezoelectric polarizations has stimulated many experimental and theoretical works [4–7]. These studies show that the electronic, dielectric and optical properties of the WZ GaN/AlGaN quantum heterostructures are strongly affected by the built-in electric field (MV/cm). However, spontaneous polarization fields do not exist in the ZB III-nitrides due to the higher crystal symmetry, and piezoelectric fields are negligible due to the (0 0 1) growth direction of epitaxial layers [8]. Thus, one of the distinguished physical properties of ZB GaN/AlGaN quantum heterostructures is the absence of the built-in electric field. And the band gap of ZB GaN is smaller than that of WZ GaN. Therefore, ZB GaN/AlGaN quantum heterostructures have attracted increasing attention because they are expected to have possible advantages for optoelectronic applications [9–12].

It is well known that impurity states play a very important role in the semiconductor optoelectronic devices. Without impurities, there would be no diode, no transistor, or any semiconductor science and technology. A deep understanding of the effects of impurities on electronic states of semiconductor quantum heterostructures is a fundamental question in semiconductor physics because their presence can dramatically alter the performance of quantum devices [13]. In the past many years, there have many theoretical investigations on the binding energy of hydrogenic impurities in GaAs/AlGaN and InAs/GaAs low dimension quantum structure [14–19]. These studies show that the binding energy of hydrogenic impurities in nanoscopic systems depends upon materials and geometry (size and shape) and impurity position. To the best of our knowledge, there are no theoretical and experimental investigations on hydrogenic impurity states in ZB GaN quantum dot (QD). In order to understand the impurity states in the ZB GaN/AlGaN QD, we will investigate the binding energy of a hydrogenic donor

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doi:10.1016/j.mejo.2007.06.003

impurity in ZB GaN/AlGaN cylindrical QD using a variational procedure.

The present paper is organized as follows. In Section 2, we give a simple theoretical model to investigate hydrogenic impurity states in ZB GaN/AlGaN QD. Numerical results for the binding energy of a hydrogenic donor impurity in the ZB GaN/AlGaN QD are given and discussed in Section 3. Finally, we summarize the main conclusions obtained in this paper in Section 4.

2. Theoretical model

According to previous studies on ZB GaN QD [9], for simplicity, we consider a hydrogenic donor impurity in a cylindrical ZB GaN QD with radius R and height L, surrounded by large energy gap materials ZB $Al_xGa_{1-x}N$, in which the origin is taken at the center of the QD and the z axis is defined to be the growth direction (see Fig. 1).

Within the framework of effective-mass approximation, the Hamiltonian for a hydrogenic donor impurity in the cylindrical ZB GaN/AlGaN QD may be written as

$$\hat{H} = \hat{H}_0 - \frac{e^2}{4\pi\varepsilon_0\bar{\varepsilon}r}, \tag{1}$$

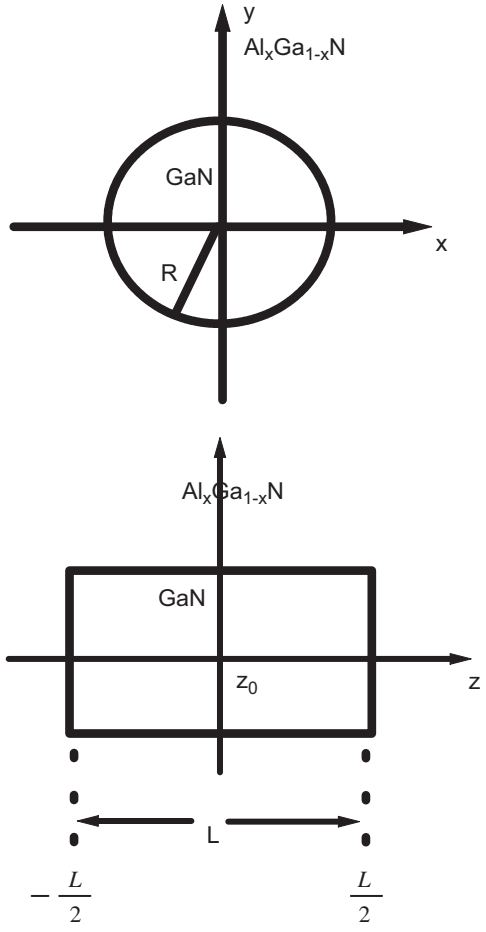

Fig. 1. A diagram of a cylindrical ZB GaN QD with the radius R and the height L, surrounded by the large energy gap materials ZB $Al_xGa_{1-x}N$.

with

$$\hat{H}_0 = -\frac{\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} - \frac{\partial^2}{\partial z^2}\right] + V(\vec{r}), \tag{2}$$

where $r = \sqrt{(x-x_i)^2 + (y-y_i)^2 + (z-z_i)^2}$ is the distance between the electron and the impurity site, $x(x_i)$, $y(y_i)$ and $z(z_i)$ are the coordinates of the electron (impurity) in the QD, e is the absolute value of the electron charge, ε_0 is the permittivity of free space, and $\bar{\varepsilon}$ is the effective mean relative dielectric constant of the embedding material, m^* is the electron effective mass, $V(\vec{r})$ is confinement potential due to the conductor band offset in the ZB GaN/AlGaN QD.

In order to calculate the energy of the hydrogenic donor impurity in the ZB GaN/AlGaN QD, the trial wave function may be written as

$$\Phi = \psi(\rho,\varphi,z)e^{-\alpha\rho_{ei}^2-\beta z_{ei}^2}, \tag{3}$$

where $\psi(\rho,\varphi,z)$ is the eigenfunction of the Hamiltonian described in Eq. (2). The exponential term in Eq. (3) accounts for the presence of the hydrogenic impurity, α and β are variational parameters. $\rho_{ei}^2 = (x-x_i)^2 + (y-y_i)^2$ and $z_{ei}^2 = (z-z_i)^2$.

If we assume that the in-plane and on-axis motions of the electron are weakly coupled, the wave function $\psi(\rho,\varphi,z)$ can be written as

$$\psi(\rho,\varphi,z) = f(\rho)h(z)e^{im\varphi}, \quad m = 0, \pm1, \pm2, \ldots, \tag{4}$$

where m is the electron z-component angular momentum quantum number. The radial wave function $f(\rho)$ can be obtained using the m-order Bessel function J_m and the modified Bessel function K_m. The z-axis wave function $h(z)$ can be obtained using linear combinations of analytical functions $\sin(\xi)$ and $\cos(\xi)$ (dot), or $\exp(\xi)$ (barriers).

The energy of a hydrogenic donor impurity in the ZB GaN/AlGaN QD may be obtained by minimizing

$$E = \min_{\alpha,\beta}\frac{\langle\Phi|\hat{H}|\Phi\rangle}{\langle\Phi|\Phi\rangle}. \tag{5}$$

The donor binding energy E_b can be represented as follows:

$$E_b = E_0 - E, \tag{6}$$

where E_0 is the energy for the Hamiltonian of Eq. (2).

3. Numerical results and discussion

We have calculated the donor binding energy E_b as functions of the impurity position and QDs structural parameters, such as dot height L, radius R and In content x of ZB InGaN material. All material parameters used in this paper are the same as in Ref. [9].

In Fig. 2, the donor binding energy E_b is investigated as a function of the impurity positions z_i and ρ_i in the ZB GaN/AlGaN QD. Fig. 2 shows that the donor binding energy E_b has a maximum value when the impurity is located at the center of the QD. The reason is that the