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Pressure-dependent shallow donor binding energy in InGaN/GaN square QWWs

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ABSTRACT

Using a variational approach, we perform a theoretical study of hydrostatic pressure effect on the ground-state of axial hydrogenic shallow-donor impurity binding energy in InGaN/GaN square quantum well wire (SQWWs) as a function of the side length within the effective-mass scheme and finite potential barrier. The pressure dependence of wire length, effective mass, dielectric constant and potential barrier are taken into account. Numerical results show that: (i) the binding energy is strongly affected by the wire length and the external applied pressure and (ii) its maximum moves to the narrow wire in particular for height pressure.

1. Introduction

Recently, the physics of low-dimensional systems such quantum wells (QWs), quantum well wires (QWWs) and quantum dots (QDs) have been widely studied which is due to a dramatic change in the behavior of electrons (or holes) in semiconductor nanostructures in particularly for GaAs, PbS, PbSe, CdS and ZnO systems [1–10]. Using quantum confinement effect in these structures, one can design high quality electronic and optoelectronic devices. Therefore wide band gap group III-nitrides based semiconductor heterostructures like (In,Ga)N, (Al,Ga)N and (Al,In,Ga)N have attracted much interest. These materials are most promising for high-power, high-temperature electronic devices, such as high-brightness blue–green light emitting diodes (LEDs) and laser diodes (LDs) which is due to their direct and large band gap ranging from infrared to ultraviolet emission [11–13]. Our purpose is to expand these studies to (In,Ga)N/GaN low dimensional systems and compare our results to those reported by Baser et al. which concern the cylindrical quantum-well wire (CQWW) system [14,15].

In the present study, we have used a variational procedure of the hydrogenic-type trial wave-function within the effective-mass approximation to investigate the hydrostatic pressure effect on shallow donor impurity binding energy of InGaN/GaN square quantum-well wire (SQWW).

2. Theoretical framework

We consider on-center shallow-donor impurity in the square quantum well wire (SQWW) made of (In,Ga)N and embedded in GaN barrier. In this case, it is convenient to use the Cartesian coordinates. In the framework of effective-mass approximation without electron–phonon interaction and spin–orbit coupling, the Hamiltonian for rectangular cross-section wire, lying along z-axis, is given as follows:

$$H_0 = -(\hbar^2/2m^*(P))[d^2/dx^2 + d^2/dy^2] + V_C \tag{1}$$

$m^*(P)$ is the pressure-dependent electron effective-mass in the wire and the barrier regions defined as follows:

$$m^*(v,P) = \begin{cases} v m^*_{e,\mathrm{InN}} + (1-v) m^*_{e,\mathrm{GaN}} & |x| \le L(P)/2 \text{ and } |y| \le L_0/2 \\ m^*_{e,\mathrm{GaN}} & \text{elsewhere} \end{cases} \tag{2}$$

The electron effective-mass is equal to $0.19m_0$ ($0.1m_0$) in GaN (InN), m_0 is the free electron mass, V_C is the barrier potential expressed as:

$$V_C = \begin{cases} 0 & |x| \le L(P)/2 \text{ and } |y| \le L_0/2 \\ V_0(v,P) & \text{elsewhere} \end{cases} \tag{3}$$

$V_0(v,P)$ denotes the conductor band offset. Following the recent study reported by Schulz and Reilly [16], the band offset $\Delta E_C : \Delta E_V$ is taken to be 70:30. Then $V_0(v,P)$ can be expressed as:

$$V_0(v,P) = 0.7\,[E_g^{\mathrm{GaN}}(P) - E_g^{\mathrm{InGaN}}(P)] \tag{4}$$

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The GaN (InN) band gap energy pressure-dependence used in this paper is the same as that given in Ref. [17] which can be expressed as follows:

$$E_g(P) = E_g(0) + \left(\gamma P + \delta P^2\right) \quad (5)$$

$E_g(0)$ is the GaN (InN) band gap energy without the pressure effect. It is equal to 3.22 (0.77) eV at room temperature while the pressure coefficients of GaN (InN) are $\gamma = 40\,(16)$ meV/GPa and $\delta = -0.38\,(-0.02)$ meV/GPa^2.

Several experimental and theoretical studies concerning the band gap energy of the (In,Ga)N ternary alloy are reported in the literature. It is governed by the indium fraction (v) and it is given by the following formulas:

$$E_g^{InGaN}(v) = vE_g^{InN} + (1-v)E_g^{GaN} - bv(1-v)\ (\text{eV}) \quad (6)$$

b is the bowing parameter taking account of band gap non-linearity as a function of the indium composition. We have used the value ($b=3.8$) as reported in the recent work [18].

We notice that the pressure is applied among the x-axis and then the $L(P)$ length pressure dependence is given [19] as follows:

$$L(P) = L_0[1-3(S_{11}+S_{12})P] \quad (7)$$

The S_{ij} coefficients are the elastic compliance constants. They can be obtained using the results reported in Ref. [20] concerning the elastic constant of GaN (InN) given respectively as 293 (1 8 7) GPa and 159 (1 2 5) GPa. $L_0$is the side length without the pressure effect.

Taking account of the impurity located at $M_0(x_0,y_0,z_0)$, the Hamiltonian equation (Eq. (1)) becomes:

$$H = H_0 - \frac{\hbar^2}{2m^*(P)}\frac{d^2}{dz^2} - \frac{e^2}{4\pi\varepsilon_0\varepsilon_r(P)\sqrt{(x-x_0)^2+(y-y_0)^2+(z-z_0)^2}} \quad (10)$$

$\varepsilon_r(P)$ is the relative dielectric constant pressure dependency given as:

$$\varepsilon_r(P) = \begin{cases} v\varepsilon_r^{InN} + (1-v)\varepsilon_r^{GaN} & |x| \le L(P)/2 \text{ and } |y| \le L_0/2 \\ \varepsilon_r^{GaN} & \text{elsewhere} \end{cases} \quad (11)$$

The mean dielectric constant is equal to 9.8 (13.7) for GaN (InN).

In this case, analytical solution cannot be obtained, so we have used a variational approach. The trial function used for the ground-state is:

$$\psi(x,y,z,P) = N\psi_0(x,y,P)\ \exp\left[-\lambda\sqrt{(x-x_0)^2+(y-y_0)^2+(z-z_0)^2}\right] \quad (12)$$

λ is a variational parameter, N is the normalization constant and ψ_0 is the ground state wave-function obtained without the presence of the impurity. It is given as:

$$\psi_0(x,y,P) = \begin{cases} \exp[\alpha(x+y)] & x \prec -L(P)/2 \text{ and } y \prec -L_0/2 \\ \cos(\beta x)\cos(\beta y) & |x| \le L(P)/2 \text{ and } |y| \le L_0/2 \\ \exp[-\alpha(x+y)] & x \succ L(P)/2 \text{ and } y \succ L_0/2 \end{cases} \quad (13)$$

$$\alpha^2 = \frac{2m^*}{\hbar^2}[V_0(P) - E_0] \quad (14)$$

and

$$\beta^2 = \frac{2m^*E_0}{\hbar^2} \quad (15)$$

Taking account of the boundary conditions, we have obtained:

$$\alpha^2 = \beta^2\frac{1-\cos(\beta L)}{1+\cos(\beta L)} \quad (16)$$

The energy is obtained by minimization with respect to the variational parameters λ. Then, the binding energy of shallow donor impurity is deduced from those of the ground-state energy of an electron in SQWW with and without the presence of the impurity. It is given by the following expression:

$$E_b(v,P) = E_0 - \min_{\lambda}\frac{\prec\psi\left(\vec{r}\right)|H|\psi\left(\vec{r}\right)\succ}{\prec\psi\left(\vec{r}\right)|\psi\left(\vec{r}\right)\succ} \quad (17)$$

E_0 is the ground-state energy in the absence of the impurity.

3. Results and discussion:

Our results are presented in the effective units without pressure effect, $R_y = m^*e^4/2\hbar^2\varepsilon_r^2$ for the energy (27.48 meV for GaN, 12.22 meV for InN and 26.65 meV for $In_{0.2}Ga_{0.8}N$) and $a_B = \varepsilon_r\hbar^2/m^*e^2$ for the length (2.70 nm for GaN, 6.10 nm for InN and 2.80 nm for $In_{0.2}Ga_{0.8}N$).

To understand the pressure effect, we have primarily investigated the potential barrier dependence of pressure of the SQWW for different indium concentrations at room temperature. Fig. 1 shows that the potential barrier increases with the increase in the pressure. This increase is more significant for high indium fraction. This behavior can be explained by the band gap pressure dependence. From the values reported in Ref. [13], one can see that the decrease of the band gap energy as a function of the hydrostatic pressure of $In_vGa_{1-v}N$ is more significant than that of GaN. This effect raises relatively the potential barrier, enhances the confinement effect and reduces the wave-function expansion across the barrier which affects the shallow-donor binding energy.

Secondly, we have calculated the binding energy for an on-center shallow donor placed in InGaN/GaN SQWW under hydrostatic pressure for different indium fractions at room temperature. The results are obtained for different indium concentrations (10%, 20%, 30% and 40%). We remark that the binding energy shape is the same and increases as a function of the indium concentration; however its maximum moves to narrow wire when the indium fraction increases. In Fig. 2, we present only the results obtained for 20%. One can see that the binding energy increases as a function of the pressure for all lengths. This increase is more important for a pressure equal to 40 GPa. It is found that the binding energy does not increases linearly with

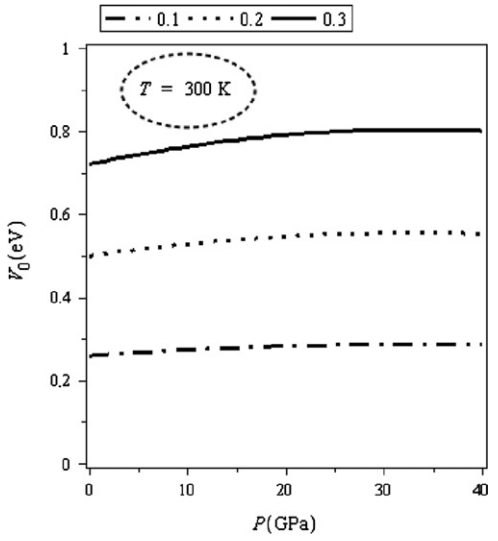

Fig. 1. The potential barrier as a function of hydrostatic pressure in $In_vGa_{1-v}N$/GaN SQWW at room temperature for three indium fractions.