Superlattices and Microstructures 48 (2010) 298–304

Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

Simultaneous effects of hydrostatic pressure and temperature on the binding energy of hydrogenic impurity in cylindrical quantum well wires

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ARTICLE INFO

Article history:
Received 25 March 2010
Received in revised form
24 June 2010
Accepted 25 June 2010
Available online 3 August 2010

Keywords:
Hydrostatic pressure
Impurity and defect levels
Energy states of adsorbed species
Quantum wells
Quantum wires

ABSTRACT

The effect of hydrostatic pressure and temperature on the ground state binding energy of hydrogenic impurities is investigated in a $GaAs/Ga_{0.7}Al_{0.3}As$ cylindrical quantum well wire as a function of the wire radius. The calculations are performed using a variational procedure within the effective mass approximation for a finite confinement potential for various values of the hydrostatic pressure and temperatures. The results are compared with the available data in literature and found to be in a good agreement with them.

1. Introduction

In the last three decades, there have been tremendous research activities on low-dimensional semiconductor systems powered by the advances in crystal growth and processing techniques, such as molecular-beam epitaxy (MBE), metal–organic chemical–vapour deposition (MOCVD) and advanced lithography, which made it possible to confine electrons in extremely thin semiconducting wires, namely, quantum well wires with nano dimensions. The confinement driven electronic and optical properties of superlattices and heterostructures and their wide range of potential device applications have made them one of the most studied materials for both experimental and theoretical studies. Therefore, these structures have been used experimentally to study the physical properties of low dimensional systems and their quantum effects, while several theoretical calculations on these systems have been performed and compared with experimental results to explore their excitonic and impurity binding energies, electronic and optical structures, transport properties, etc. [1–20].

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doi:10.1016/j.spmi.2010.06.021

Brown and Spector calculated the hydrogenic impurity binding energies for arbitrary impurity positions using infinite and finite cylindrical confining potentials in QWWs [21]. Correa et al. studied the hydrostatic pressure effects on the donor impurity related photo ionization cross-section in cylindrical shaped GaAs/$Ga_{0.7}Al_{0.3}As$ QWWs [22]. A.J. Peter and Karki et al. reported the ground state binding energy of hydronic donors in cylindrical quantum wire under a uniform external magnetic field applied to the wire axis. Karki et al. also extended this study including barrier height effects under a uniform external magnetic field [23,18]. Peter and Navaneethakrishnan worked out the ground state and a few excited state energies of a hydrogenic donor in a quantum well under low hydrostatic pressures including temperature effects [24].

In this work, the ground state binding energy has been investigated on pressure and temperature value dependencies as a function of wire radius by using variational calculations within the effective-mass approximation in GaAs/$Ga_{0.7}Al_{0.3}As$ QWWs. The calculations are made for a cylindrical quantum wire system made as a core wire, made of GaAs embedded in $Ga_{0.7}Al_{0.3}As$ with a spatial cylindrical quantum well wire confinement. The results are then compared with existing data available. The calculation method followed is presented in Section 2 while the results and discussion are provided in the Section 3.

2. Theory

In the effective-mass approximation, Hamiltonian for a hydrogenic impurity under the effects of hydrostatic pressure and temperature in a single GaAs/(Ga, Al)As cylindrical quantum wire is written by

$$H = \frac{\hbar^2}{2}\vec{\nabla}\left(\frac{1}{m^*_{w,b}(P,T)}\vec{\nabla}\right) - \frac{e^2}{\varepsilon_{w,b}(P,T)|\vec{r}-\vec{r}_o|} + V(z,P,T), \tag{1}$$

where P is the hydrostatic pressure in GPa and T is the temperature in Kelvin. In the above equation, $|\vec{r}-\vec{r}_o| = \sqrt{\rho^2+\rho_o^2-2\rho\rho_o\cos(\phi-\phi_o)+z^2}$ is the separation of the electron–impurity ion pair and the z coordinate denotes the relative separation of the electron–impurity ion along the wire axis. $V(z,P,T)$ is the spatial confinement potential. The subscripts w and b stand for quantum wire layer GaAs and barrier layer (Ga, Al)As materials, respectively. The application of pressure and temperature modify the lattice constants, barrier height, wire sizes, effective masses and dielectric constants. The $m^*_{w,b}(P,T)$ are the corresponding effective masses in the quantum wire layer and barrier layer as a function of pressure and temperature, respectively. These are defined by

$$\begin{aligned} m^*_w(P,T) &= \left[1+7.51\left(\frac{2}{E_g(P,T)}+\frac{1}{E_g(P,T)+0.341}\right)\right]^{-1} m_o \\ m^*_b(P,T,x) &= m^*_w(P,T)+0.083m_o x \end{aligned} \tag{2}$$

where m_o is free electron mass and x is the mole fraction of aluminum in $Ga_{1-x}Al_xAs$ barrier layer. In our case, the aluminum concentration is taken to be 0.3. In the above expression, $m^*_b(P,T,x)$ is the corresponding conduction effective mass in the barrier layer, which is obtained, from a linear interpolation between the GaAs and AlAs compounds [25,26]. $E_g(P,T)$ is the variation of the energy band gap for a GaAs quantum wire at Γ-point with hydrostatic pressure and temperature. This is written as

$$E_g(P,T) = E_g(0,T) + bP + cP^2 \tag{3}$$

where $b = 1.26\times10^{-1}$ eV GPa^{-1} and $c = -3.77\times10^{-3}$ eV GPa^{-2} and

$$E_g(0,T) = \left[1.519 - 5.405\times10^{-4}\frac{T^2}{T+204}\right] \text{ eV}. \tag{4}$$

In Eq. (1), $\varepsilon_{w,b}(P,T)$ are the hydrostatic pressure and temperature dependent dielectric constants of the wire and barrier layer respectively. In our calculations, the charge image effects have not been