HYDROSTATIC PRESSURE AND TEMPERATURE EFFECTS ON THE DONOR BINDING ENERGY IN ASYMMETRICAL SQUARE QUANTUM WELLS

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In lucrare se prezintă efectele presiunii şi ale temperaturii asupra energiei de legătură pentru donori puțin adânci situați în gropi cuantice asimetrice din GaAs/AlGaAs. Calculele sunt făcute în aproximația masei efective, folosind o metodă variațională. Se constată că efectele asimetriei, presiunii şi temperaturii sunt accentuate în structuri cuantice cu o confinare puternică a purtătorilor.

We calculated the effects of the hydrostatic pressure and temperature on the binding energy for centric shallow donors in asymmetrical GaAs/AlGaAs quantum wells, within the effective mass approximation and variational approach. We found that the pressure, temperature and asymmetry effects are mainly observed when the quantum confinement due to the barrier potential are stronger.

Keywords: asymmetrical quantum wells, pressure effect, binding energy

1. Introduction

In recent years semiconductor quantum well (QW) structures have attracted much attention due to their novel electronic and optical properties [1-9].

The optical properties of these type of nanostructures mainly depend on the asymmetry of the confining potential. Such an asymmetry can be obtained either by applying an electric field to a symmetric QW or by compositionally grading the QW. Recently, Karabulut *et al*. [10] studied the linear and nonlinear optical absorptions in an asymmetrical rectangular QW.

In this paper we investigated the effects of the hydrostatic pressure and temperature on the electronic states and donor binding energy in a GaAs/AlGaAs compositionally asymmetric square QW (ASQW). This QW structure has a tunable degree of asymmetry resulting in promising nonlinear optical properties. We found that for a narrow well the dependence of the binding energy on the hydrostatic pressure and asymmetric parameter are more pronounced.

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2. Theory

We consider an ASQW composed of three different semiconductor layers located at $z < -L/2$ (left layer), $-L/2 \le z \le L/2$ (QW layer), and $z > L/2$ (right layer). In the effective mass approximation, the Hamiltonian for an on-center hydrogenic donor impurity in a QW, having the *z*-axis as the growth direction, under action of hydrostatic pressure is given by

$$H = \frac{P_{\perp}^2}{2m_{w,b}^*(p,T)} + V_z(p,T) + V_C(\vec{r},p,T). \tag{1}$$

Here $P_{\perp}^2 / 2m_{w,b}^*(p,T)$ is the kinetic energy operator in the *x*-*y* plane, *p* is the hydrostatic pressure in kbar, *T* is the temperature in Kelvin. The subscripts *w* and *b* stand for the well and barrier layer materials, respectively.

The application of hydrostatic pressure modifies the barrier height, effective masses $m_{w,b}^*(p,T)$, and dielectric constants. The expression for $m_w^*(p,T)$ [11] is

$$\frac{m_0}{m_w^*(p,T)} = 1 + E_p^{\Gamma}\left[\frac{2}{E_g^{\Gamma}(p,T)} + \frac{1}{E_g^{\Gamma}(p,T)+\Delta_0}\right]. \tag{2}$$

Here m_0 is the free electron mass, E_p^{Γ} = 7.51 eV is the energy related to the momentum matrix element, Δ_0 = 0.341 eV is the spin-orbit splitting, and $E_g^{\Gamma}(p,T)$ is the pressure- and temperature-dependent energy gap for the GaAs QW at the Γ-point [12]. The expression for $E_g^{\Gamma}(p,T)$ is

$$E_g^{\Gamma}(p,T) = E_g^{\Gamma}(0,T) + bp + cp^2 \tag{3}$$

where $E_g^{\Gamma}(0,T) = 1.519 - \left(5.405\times10^{-4}T^2\right)/\left(T+204\right)$, b = 0.0126 eV/kbar, and c = 3.77×10^{-5} eV/(kbar)^2. The corresponding conduction effective masses in the two barriers are obtained from a linear interpolation between the GaAs and AlAs compounds [11, 13], i.e.

$$m_b^*(p,T) = m_w^*(p,T) + 0.083x\,m_0 \tag{4}$$

where *x* is the Al concentration in the layer.

$V_z(p,T)$ is the confining potential defined as:

$$V_z(p,T) = \begin{cases} V_l, & z < -L/2 \\ 0, & -L/2 \le z \le L/2 \\ V_r, & z > L/2 \end{cases}. \tag{5}$$

Here V_l and V_r are the left and right barrier height, respectively, and L is the QW width. This asymmetric potential is generated by the three layers with different Al mole fractions x_i (i = l, 0, r). We define the asymmetry parameter $\beta = x_r / x_l$. Under the applied pressure the barrier heights are given by

$$V_i(p,T) = Q_c \Delta E_g^{\Gamma}(x_i, p, T), \ (i = l, r) \ . \tag{6}$$

Here Q_c = 0.658 is the conduction band offset parameter and $\Delta E_g^{\Gamma}(x_i, p, T) = \Delta E_g^{\Gamma}(x_i) + D(x_i)p + G(x_i)T$ with parameters defined in Ref. [13].

The quantity $V_C(\vec{r}, p, T)$ is the Coulomb potential [15] given by

$$V_C(\vec{r}, p, T) = -\frac{e^2}{4\pi\varepsilon_{w,b}(p,T)\cdot r} \ . \tag{7}$$

The dielectric constant $\varepsilon_w(p,T)$ in the well region [16] is defined as

$$\varepsilon_w(p,T) = \begin{cases} 12.74\, exp\left(-1.73\cdot 10^{-3} p\right) exp\left[9.4\cdot 10^{-5}(T-75.6)\right]; & T \le 200\, K \\ 13.18\, exp\left(-1.73\cdot 10^{-3} p\right) exp\left[20.4\cdot 10^{-5}(T-300)\right]; & T \ge 200\, K \end{cases} \ . \tag{8}$$

The corresponding dielectric constants in the two barriers are obtained by linear interpolation between the GaAs and AlAs compounds [13]

$$\varepsilon_b(p,T) = \varepsilon_w(p,T) - 3.12x \ . \tag{9}$$

In order to get the impurity binding energy, we use a variational method and we consider the following trial wave function

$$\Psi(\rho, z, \lambda) = \phi_0(z) \exp\left[-\rho / \lambda\right] \tag{10}$$

where λ is the variational parameter and $\phi_0(z)$ is the eigenfunction of the Hamiltonian in Eq. (1) without the impurity potential term. The envelope wave function $\phi_0(z)$ is

$$\phi(z) = \begin{cases} A\exp(ik_l z), & z < -L/2 \\ B\sin(kz) + C\cos(kz), & -L/2 \le z \le L/2 \\ D\exp(-ik_r z), & z > L/2 \end{cases} \tag{11}$$

where $k_i = \sqrt{2m_i^*(V_i - E_0)}/\hbar$, i = l, r and $k = \sqrt{2m_w^* E_0}/\hbar$. The constants A-D and the subband energy E_0 are obtained form the continuity of the wave function.

The ground-state impurity binding energy is given by

$$E_b(p,T) = E_0(p,T) - \min_{\lambda} \frac{\langle \Psi | H \Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{12}$$

where $E_0(p,T)$ is the lowest subband energy related to the $\phi_0(z)$ wave function.

3. Results and discussion

In numerical calculations we used x_l = 0.3 and a variable x_r.

Fig.1 presents the variation of the lowest subband energy with hydrostatic pressure for different values of the asymmetry parameter β and two QW widths L = 5 nm and L = 20 nm, at T = 4 K and T = 300 K.

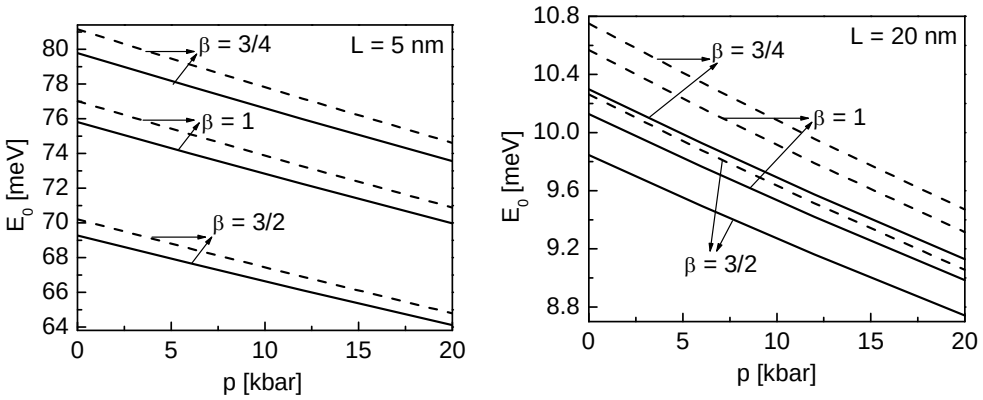

Fig.1 The variation of the lowest subband energy with hydrostatic pressure for different values of the parameter β and two QW widths, at T = 4 K (solid lines) and T = 300 K (dashed lines).

We note that the lowest subband energy E_0 linearly decreases with hydrostatic pressure p for all the cases under our investigation, as expected. This is due to the reduction of the barrier heigths under action of the hydrostatic pressure and temperature (Eq. (7)). The decreasing of the ground energy level E_0 under pressure action is more obvious for a narrow QW. For example, the slope of the dependence $E_0(p)$, $|s|$, at T = 300 K, varies between 0.271 meV/kbar (β = 3/2) and 0.327 meV/kbar (β = 3/4) for a 5 nm width ASQW. Instead, for a wider QW (L = 20 nm) $|s|$ varies between 0.060 meV/kbar (β = 3/2) and 0.064 meV/kbar (β = 3/4). This behavior is in agreement with previous works [6, 8].

Also, as the asymmetry parameter decreases the electron confinement in the QW structure becomes more pronounced leading to an augmentation of the subband energy levels (push-up effect, Fig.1). As expected, the increasing of the QW size results in the diminution of the ground energy level.

Fig.2 shows the variation of the donor binding energy E_b on the hydrostatic pressure for different values of the asymmetry parameter β, in two ASQWs with L = 5 nm and 20 nm, at T = 4 K and T = 300 K.

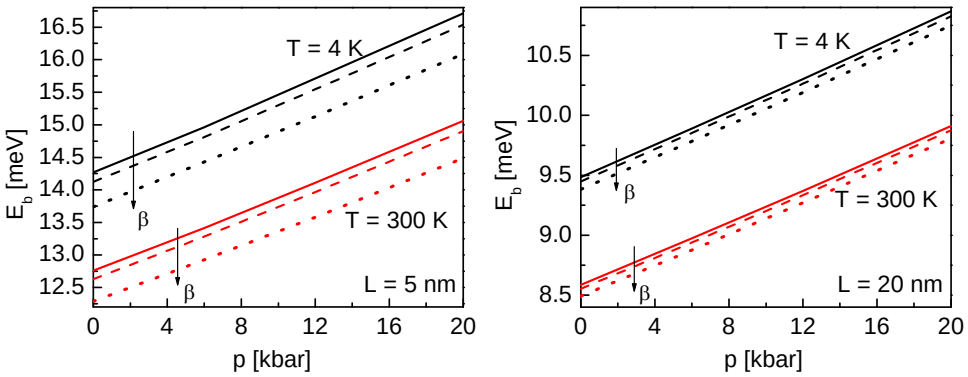

Fig.2 Donor binding energy vs. hydrostatic pressure for different values of the asymmetry (β =3/4, solid line; β = 1, dashed line; β = 3/2, dotted line), for two ASQWs, at T = 4 K and T = 300 K.

We observe that E_b linearly increases with hydrostatic pressure, as expected [8]. This behavior reflects the additional confinement due to the reduction of the dielectric constants (Eq. (8)). The slope *s'* of the dependence $E_b(p)$ varies between 0.11 meV/kbar (β = 3/2, T = 300 K) and 0.12 meV/kbar (β = 3/4, T = 4 K) for a 5 nm width ASQW. In a wider QW (L = 20 nm) *s'* is almost independent of β and T, *s'* ≅ 0.07 meV/kbar.

In Fig.3 we present the binding energy dependence on the asymmetry parameter β for different values of the hydrostatic pressure p, for two ASQWs with L = 5 nm and 20 nm, at T = 4 K and T = 300 K.

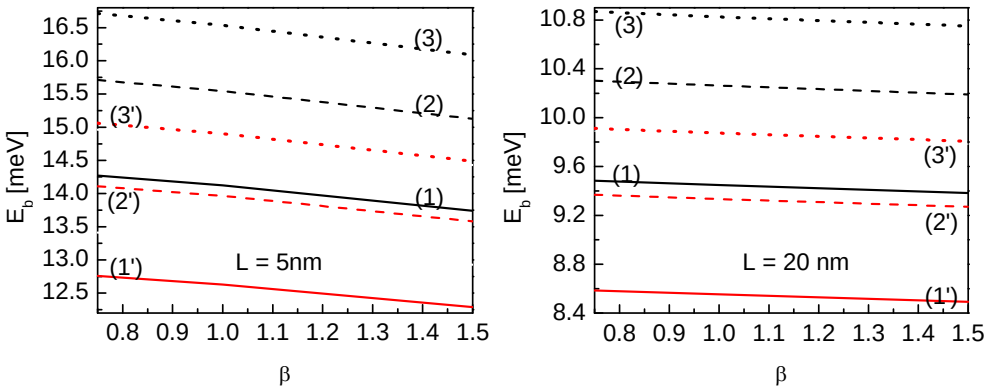

Fig.3 Donor binding energy vs. asymmetry parameter β for different values of the hydrostatic pressure p, for two ASQWs. Numbers 1, 2 and 3 stand for p = 0, 12 kbar and 20 kbar, respectively, at T = 4 K; 1', 2' and 3' stand for T = 300 K.

Similar to ground energy level E_0 case the reduction of the confinement induced by the increasing of the asymmetry parameter β and temperature T results in the diminution of the donor binding energy.

4. Conclusions

Using the effective mass approximation, we have calculated the ground state energy of a hydrogenic donor in an asymmetrical GaAs/AlGaAs QW as a function of the hydrostatic pressure, asymmetry parameter and temperature for two well widths. We found that for a narrow well the dependencies of the binding energy on the hydrostatic pressure and asymmetric parameter are more pronounced. The hydrostatic pressure effect is essentially associated with the dielectric constant decreasing and a corresponding increasing in the Coulomb interaction and donor binding energy. These results may have important consequences for optical studies on semiconductor QWs and offers a new degree of freedom in designing optoelectronic devices.

R E F E R E N C E S

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