DONOR BINDING ENERGY IN DIELECTRIC GRADED GaAs-(Ga, Al)As QUANTUM-WELL WIRES

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ABSTRACT
The results obtained previously for the ground state of the shallow donor centered in quantum-well wires GaAs-(Ga, Al)As (QWW) with a gradual variation of the of the *Al* concentration in a thin interface layer at the junction is extended to the model that takes into account the effective-mass and the dielectric constant dependencies on the *Al* concentration, given by a linear interpolation formulae. To find the electrostatic energy in a dielectric QWW the Poisson equation is solved by using the first order perturbation theory. The ground state binding energy of a donor centered in a GaAs-(Ga, Al)As QWW, as a function of the wire radius is calculated by using the trigonometric sweep method. A considerable enhancement of the binding energy in comparison with results obtained previously is found.

INTRODUCTION
With the advancement of molecular-beam epitaxy as a technique that permits to grow wire-like compound semiconductor structures of low nanometer size a great deal of attention has been the theoretical study of the hydrogenic impurity states in these quasi-one-dimensional systems [1-4]. However, in these studies the dependence of the dielectric constant and effective mass on the heterostructure composition are neglected. Previously, several researchers have analyzed the effect of the material parameters mismatch inside and outside the quantum well (QW) [5,6] and quantum dot (QD) [7] and have been found that this effect is important. The model with the abrupt variation of the conduction band edge position, electron effective mass and the dielectric constant in the interfaces has been considered for QW [5,6] and the increase produced by material parameters mismatch up to 20% for a narrow has been found. A more general model, that include not only abrupt but also slowly varying the conduction band edge position and the material parameters, has been proposed early for QD [7]. In this work, the last model is extended to analyze the effect of the confining potential shape and the material parameters variation on the ground state binding energy of a donor located at the axis of symmetry in a cylindrical GaAs/$Ga_{1-x}Al_xAs$ quantum well wire. To find the electrostatic potential produced by donor in the heterostructure with variable dielectric constant we use the first order perturbation theory for Green function and to solve the one-dimensional Schrödinger equations the numerical trigonometric sweep procedure [8].

MODEL
We consider a model of the cylindrical GaAs/$Ga_{1-x}Al_xAs$ QWW of radius R with a smooth increasing of the *Al* concentration in the radial direction, according to relation:

$$c(\rho) = x\frac{1-\exp(-\rho/\xi)}{1+\exp[-(\rho - R)/\xi]}, \tag{1}$$

where ρ is a distance from the QWW axis, x is a respective value of the *Al* concentration in the barrier and the parameter ξ can be associated wit the thickness of the transition region in the junction. It is seen that $c(\rho)$ increases from 0 at the axis of the wire ($\rho \to 0$), up to x in the barrier as $(\rho - R)/\xi$ □1. Different shapes of the *Al* concentration distribution can be obtained, varying in this relation, the dimensionless ratio ξ / R, from almost rectangular when $\xi / R \to 0$, to a very smooth one as $\xi / R \to 1$. We assume that the variation of the position of the conduction band edge and material parameters in GaAs/$Ga_{1-x}Al_xAs$ QWW follows to the *Al* concentration change in the radial direction and we describe the dependencies of the confining potential $V(\rho)$, dielectric constant $\varepsilon(\rho)$ and effective mass $m(\rho)$ on the *Al* concentration by means of the following interpolation relations [5]:

$$\begin{aligned} &V(\rho) = 0.65\{1.087c(\rho) + 0.487c^2(\rho)\}\ (eV); \\ &\varepsilon(\rho) = \varepsilon_0\beta(\rho); \qquad \beta(\rho) = 1 - 0.218\,c(\rho); \\ &m(\rho) = m_0\eta(\rho); \qquad \eta(\rho) = 1 + 1.239\,c(\rho), \end{aligned} \tag{2}$$

where ε_0 and m_0 are the corresponding values for GaAs parameters.

The dimensionless Hamiltonian with lengths scaled in terms of the GaAs effective Bohr radius (a_0*) and the energies in the effective Rydberg (Ry*) for a neutral donor impurity located at the center of a QWW within the parabolic effective-mass approximation can be written as

$$H = H_0(\mathbf{r}) - 2U(\mathbf{r}); \quad H_0(\mathbf{r}) = -\nabla\left[\frac{1}{\eta(\rho)}\nabla\right] + V(\rho) \tag{3}$$

where H_0 is the Hamiltonian for an unbound electron in the wire, whose eigenfunction f_0, and eigenvalue E_0, for the ground state can be found exactly by solving the problem:

$$H_0 f_0(\mathbf{r}) = E_0 f_0(\mathbf{r}), \tag{4}$$

and $U(\mathbf{r})$ is the electrostatic energy of the electron-ion interaction that is solution of the Poisson equation:

$$\Delta U(\mathbf{r}) + \frac{d\beta(\rho)}{d\rho}\frac{\partial U(\mathbf{r})}{\partial\rho} = -4\pi\delta(\mathbf{r}) \tag{5}$$

THEORY

To solve the equation (5) one can use the perturbation theory considering $\xi\, d\beta / d\rho$ as a small parameter, which for example for a *Al* concentration 0.3 is of the order 0.05. The first order of the perturbation theory gives for electrostatic energy in cylindrical coordinates the following result:

$$U(\rho,z)=\frac{1}{\sqrt{\rho^2+z^2}}+U_1(\rho,z);\quad U_1(\rho,z)=-\frac{1}{4\pi}\int_0^\infty \rho'^2\frac{d\beta(\rho')}{d\rho'}F_1(\rho',\rho,z)d\rho' \tag{6}$$

where

$$F_1(\rho',\rho,z)=\int_{-\infty}^{\infty}\frac{F_2\left(2\rho\rho'/(\rho^2+\rho'^2+(z-z')^2)\right)}{\sqrt{(\rho'^2+z'^2)^3}\sqrt{\rho^2+\rho'^2+(z-z')^2}}dz';\quad F_2(x)=\int_0^\pi\frac{d\varphi}{\sqrt{1-x\cos\varphi}}$$

The Schrödinger equation (4) for a very long cylindrical wire is separable in cylindrical coordinates and the ground state wave function f_0 for the unbound electron depends only on the electron distance from the axis of symmetry, $f_0(\mathbf{r})\equiv f_0(\rho)$. Any numerical procedure, for example the exact numerical trigonometric sweep method [4,8], can be used to solve the separated one-dimensional differential equation with respect to the function $f_0(\rho)$. On the contrary, the corresponding Schrödinger's equation for the coupled electron cannot be solved exactly and therefore we have chosen a trial function in the form

$$\Psi(\mathbf{r})=f_0(\mathbf{r})\Phi(r), \tag{7}$$

where $\Phi(r)$ is a function that describes the correlation of the electron-ion motion in the QWW. Taking the functional derivative of the total energy $E[\Phi]=\langle f_0\Phi|H|f_0\Phi\rangle$ with respect the unknown function $\Phi(r)$ one can obtain the following Euler–Lagrange equation for this function:

$$-\frac{1}{S_0(r)}\frac{d}{dr}\left[S_1(r)\frac{d\Phi(r)}{dr}\right]-\left[\frac{2}{r}+\overline{U}_1(r)\right]\Phi(r)=-E_b\Phi(r);\quad E_b=E_0-E, \tag{8}$$

with E_b and E being the donor binding and ground state energies respectively and the functions $S_0(r)$, $S_1(r)$ and $\overline{U}_1(r)$ are given by the formulae:

$$S_0(r)=r^2\int_0^{2\pi}d\varphi\int_0^\pi f_0^2(r\sin\theta)\sin\theta d\theta;\quad S_1(r)=r^2\int_0^{2\pi}d\varphi\int_0^\pi\frac{f_0^2(r\sin\theta)}{\eta(r\sin\theta)}\sin\theta d\theta, \tag{9}$$

$$\overline{U}_1(r)=r\int_0^r f_0^2\left(\sqrt{r^2-z^2}\right)U_1\left(\sqrt{r^2-z^2},z\right)dz. \tag{10}$$

The one-dimensional differential equation (8) is similar to Schrödinger's equation for hydrogen atom but it includes three additional functions (9)-(10) that can be interpreted in the follow form. The function $S_0(r)$ is the volume measure function in an isotropic and non-homogeneous effective space given by the radial probability density for an unbound electron in QWW, calculated over the sphere of the radius r: As the electron-ion separation is small ($r\to 0$), the function $S_0(r)$ is parabolic $\left(S_0\sim r^2\right)$, therefore in this region the orbits of the confined impurity have a three-dimensional character. As the electron-ion distance increases the wave function in the wire interfaces vanishes and the integral becomes independent of the sphere radius, in this case the behavior is typical of a one-dimensional effective space. The other two functions $S_1(r)$ and $\overline{U}_1(r)$ are mean values of the inverse effective mass m^{-1} (**r**) and the impurity ion image potential U_1 (**r**) averaged over all direction at the surface of the sphere of radius r with center at the ion location.

RESULTS AND DISCUSSION

In Fig.1 we have plotted the curves of the ground state binding energies for D^0 center as a function of $GaAs/Ga_{0.6}Al_{0.4}As$ cylindrical QWW radius, for two different values of relative thickness of the transition region in the interface layer: ξ / R = 0.01 corresponding to the model with practically square-well confining potential and ξ / R = 0.3 corresponding to soft-edge shape of the barrier.

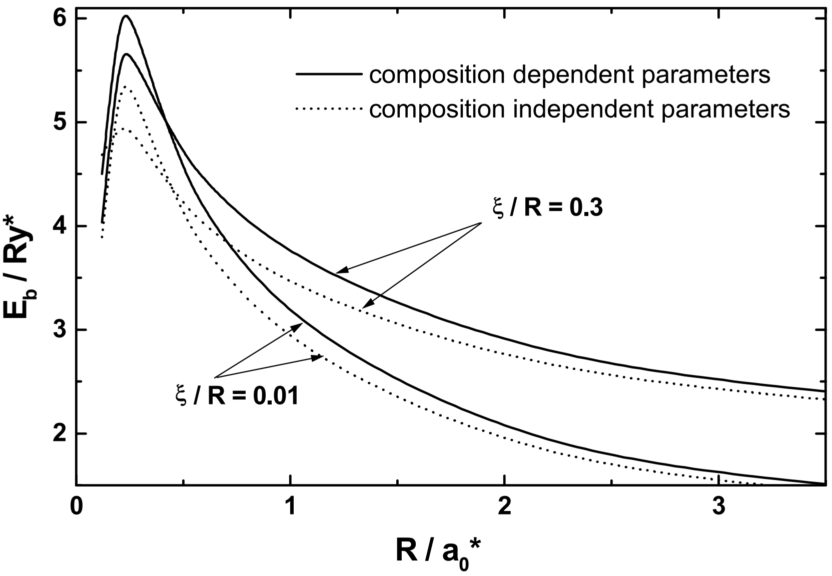

Fig.1 Ground state binding energy of a donor as the function of the radius of the cylindrical $GaAs/Ga_{0.6}Al_{0.4}As$ QWW with two different thickness of the transition region

It can be seen that the solid lines have higher binding energies than corresponding dotted lines and a difference between them is more pronounced as the QWW's radius is becomes small. Our curve for ξ / R = 0.01 and with composition independent parameters (dotted curve) is in excellent accordance with one obtained previously [2,9] for a model with rectangular shape of the confining potential.

Dependence of the effective mass and the dielectric constant on the heterostructure composition produces an increase of the binding energy in the maximum approximately from 5.40 *Ry** up to 6.05 *Ry**. These increasing can be compared with obtained previously values 0.6 *Ry** for QW [6] and 0.7 *Ry** for QD [7]. For QWW radius greater than 0.5 a_0* the potential shape smoothing leads to a noticeable increase of the binding energy due to larger confinement in this radius size range that produce QWW with smooth bottom (ξ / R = 0.3) compared to rectangular potential shape (ξ / R = 0.01) and this effect is more significant than one produced by material parameters dependence on heterostructure composition that decreases rapidly with the QWW radius increasing. On the contrary, as the QWW radius becomes smaller than 0.5 a_0* the effect of the effective mass and dielectric constant dependence on the heterostructure composition produces a greater variation of the binding energy than potential shape. Additionally, one can see the inversion of the curves of the binding energies for ξ / R = 0.3 and ξ / R = 0.01 as the QWW radius becomes smaller than 0.5 a_0* due to larger confinement in this radius size range that produce confining with rectangular shape as the energy levels are pushed up to upper part of the confining potential.

In conclusion, we have proposed a new method to analyze the effect of the material parameters dependence on the heterostructure composition and potential shape on the D^0 ground state binding energy.

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REFERENCES

[1] Bryant G.W., Phys. Rev. B **31**, 7812 (1985)
[2] S. V. Branis, G. Li, and K. K. Bajaj, Phys. Rev. B **47**, 1316 (1993)
[3] N. Porras-Montenegro, J. Phys.: Condens. Matter **5** A367 (1993)
[4] I. D. Mikhailov, R. A. Escorcia and J. Sierra-Ortega, Phys. Stat. Sol. (b) **220**, 195 (2000)
[5] T. Pang and S. G. Louie, Phys. Rev. Lett. **65**, 1635 (1990)
[6] S. Frazzoli and F. Bassani, Phys. Rev. B **41**, 5096 (1990)
[7] C. García and I. D. Mikhailov, Phys. Stat. Sol. (b) **220**, 201 (2000)
[8] F. J. Betancur, I. D. Mikhailov and L. E. Oliveira, J. Phys. D: App. Phys. 31, 3391 (1998)
[9] S. T. Pérez-Merchancano and G. E. Marques, Solid. State Commun. **110**, 209 (1999)