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The Binding Energy of Impurities in the Asymmetrical Semi-Exponential Quantum Wells

Ünal YEŞİLGÜL

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Abstract. Within the framework of effective-mass and envelope wave function approach, using a variational method, we have investigated the binding energy of shallow-donor impurities in an asymmetrical semiexponential quantum wells (ASEQW). The obtained numerical results show that the structure parameters (σ and, V₀) lead to significant changes in the impurity binding energy. Furthermore, these results show that the hydrogenic donor impurity binding energy may be increased or decreased as a function of the impurity position in quantum well.

Keywords: Quantum well, impurity.

Asimetrik Yarı-Üstel Kuantum Kuyularındaki Safsızlıkların Bağlanma Enerjisi

Özet. Etkin-kütle ve zarf dalga fonksiyonu yaklaşımı çerçevesinde, varyasyonel bir metot kullanarak, asimetrik yarı-üstel kuantum kuyularında sığ-donor safsızlıkların bağlanma enerjisini araştırdık. Elde edilen sayısal sonuçlar, yapı parametrelerinin (σ ve V₀) safsızlık bağlanma enerjisinde önemli değişikliklere yol açtığını göstermektedir. Ayrıca, bu sonuçlar, hidrojen içeren donor safsızlıkların bağlanma enerjisinin kuantum kuyusundaki safsızlık pozisyonunun bir fonksiyonu olarak arttırılabileceği veya azaltılabileceğini göstermektedir.

Anahtar Kelimeler: Kuantum kuyusu, safsızlık.

1. INTRODUCTION

Technological developments in the growth techniques in the past several years have made it possible to prepare differently formed semiconductor quantum wells (QWs). These differently shaped semiconductor structures are important because of their physical properties and technological application in electronic and optoelectronic devices. Therefore, there have been attracted considerable interests on such structures [1-12]. Li et al have studied theoretically linear and nonlinear optical properties in ASEQW [9].

Third-harmonic generation (THG) coefficients in ASEQW are studied by Mou et al. [10].

It is well known that the issue of the hydrogenic binding of an electron to a donor impurity which confined within low-dimensional is heterostructures has been a topic of considerable interest. It is important to understand the electronic and optical properties of impurities in these systems, because the optical and transport properties of the devices made of this material are strongly influenced by the presence of shallow impurities. Several studies have been done on the hydrogenic impurity in low-dimensional

* Corresponding author. *Email address:* uyesilgul@cumhuriyet.edu.tr http://dergipark.gov.tr/csj ©2016 Faculty of Science, Sivas Cumhuriyet University structures [13-20]. Sari et al. have investigated the binding energy of shallow-donor impurities in quantum-well wires (QWWs) and quantum dots (QDs) [13-16]. The problem of hydrogenic-like donor impurity, located at the center of a spherical semiconductor QD was investigated by Al-Hayek et al. [17]. Zhang et al. researched the binding energy of the shallow donor impurity in the asymmetric semiconductor QW [18]. Hydrogenlike donor impurity states in strongly oblate ellipsoidal QD have been studied by Hayrapetyan et al. [19]. Tshipa et al. have investigated the binding energies of a donor charge assumed to be located exactly at the center of symmetry of two concentric cylindrical QWWs [20]. In this work, we have investigated the binding energy of shallow-donor impurities in an ASEQW. The paper is organized as follows: in Section 2, the theoretical framework is described. Section 3 is dedicated to results and discussion. Finally, the conclusion is given in Section 4.

2. THEORY

In the effective-mass approximation, the Hamiltonian describing the interaction of an electron with a hydrogenic impurity inside a QW is given by

$$\mathbf{H} = -\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \Phi^2} \right) - \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial z^2} - \frac{e^2}{\varepsilon_0 \sqrt{(\rho)^2 + (z - z_i)^2}} + \mathbf{V}(z) \tag{1}$$

where z represents the growth direction, m^{*} is electron effective mass, e is the electron charge, the quantity ε_0 is the dielectric constant of the system, and V(z) is the confinement potentials for the electron in the z-directions. The electron confining potential, V (z), is taken as [9]

$$V(z) = \begin{cases} V_0(e^{z/\sigma} - 1) & z \ge 0 \\ \infty & z < 0 \end{cases}$$
(2)

where V_0 and σ are positive structure parameters.

Using the variational method, it is possible to associate a trial wave function, which is an approximated eigen-function of the Hamiltonian described in Eq. (1). The groundstate wave function of the impurity is given by

$$\Psi(r) = \psi(z)\phi(\rho,\lambda) \tag{3}$$

where the wave function in the (x-y) plane is

$$\phi(\rho,\lambda) = \frac{1}{\lambda} \left(\frac{2}{\pi}\right)^{1/2} Exp[-\rho/\lambda]$$
(4)

where λ is the variational parameter. The ground state donor binding energy is calculated as

$$E_{B} = E_{z} - \min_{y} \left\langle \psi \left| H \right| \psi \right\rangle \tag{5}$$

where E_z is the ground-state energy of electron obtained from the Schrödinger equation for the motion along the *z*-direction without the impurity.

3. RESULTS AND DISCUSSION

Numerical results are illustrated for a typical GaAs/AlGaAs. The values of the physical parameters used in our calculations are $m^*=$ 0.067 m₀ (m₀ is the free electron mass), $\varepsilon = 13.1$ (the static dielectric constant is assumed to be same everywhere).

In Fig. 1(a), the confinement potential profile and the initial ground state energy level with their squared wave functions for $V_0 = 40$ meV, and two different σ values is plotted. As seen in this figure, the lower σ value causes the deeper potential well, which strongly confines the electrons in the conduction band. Therefore, the initial ground state energy levels clearly shift towards higher energies with decrease in σ value.



Figure 1a. The variation of the σ value, the initial ground state and squared wave functions related to these the initial ground state in the asymmetrical semi-exponential quantum wells for $V_0 = 40$ meV as a function of the position.

In Fig. 1(b), the confinement potential profile and the initial ground state energy level with their squared wave functions for $\sigma = 5$ nm, and two different V₀ values is plotted. As seen in this figure, the higher V₀ value causes the deeper potential well, which strongly confines the electrons in the conduction band. Therefore, the initial ground state energy levels clearly shift towards higher energies with increase in V₀ value.



Figure 1b. The variation of the V₀ value, the initial ground state and squared wave functions related to these the initial ground state in the asymmetrical semi-exponential quantum wells for σ = 5 nm as a function of the position.

The variation of the binding energy as a function of the of the impurity position for $V_0 = 40 \text{ meV}$ and for different values of σ is given in Fig. 2. The figure clearly shows the reduction of the binding energy as the σ value increases. Because as the σ value decreases the geometric confinement of the donor electron increases, the probability of finding the electron around the impurity increases, and this behavior gives an increment in the donor binding energy. Furthermore, it can be observed in Fig. 2 that the variation of the binding energy with is sensitive to the impurity positon.



Figure 2. The variation of the binding energy of an impurity as a function of the impurity position for $V_0 = 40$ meV for different values of σ .

The variation of the binding energy as a function of the of the donor impurity position for $\sigma = 5$ nm and for different values of V₀ is given in Fig.3. From this figure, as the V₀ increases, the peak position of the binding energy moves to the smaller impurity position values; this is evident as the donor electron distribution shifts to the left side of the QW in the z-direction.



Figure 3. The variation of the binding energy of an impurity as a function of the impurity position for $\sigma = 5$ nm and for different values of V₀.

4. CONCLUSION

As a summary, in this study we have investigated the effects of the donor impurity position, σ and V_0 on the donor impurity binding energy in an ASEQW. The obtained results show that the structure parameters (σ and, V_0) lead to significant changes in the donor impurity binding energy. This case gives a new degree of freedom in device applications, such as near-infrared electro-absorption modulators and quantum well infrared detectors, and all optical switches.

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