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In Concentration Dependence of Shallow Impurity Binding Energy Under The Hydrostatic Pressure

Pınar Baser*, Ismail Altuntas, Sezai Elagoz

*Nanotechnology Center, Department of Physics, Cumhuriyet University, 58140 Sivas, Turkey

Abstract

The ground state binding energy of axial hydrogenic impurity in zinc-blende (ZB) $In_xGa_{1-x}N/GaN$ cylindrical quantum well wires(CQWWs) are investigated as a function of the In concentration and the radius of the wire under hydrostatic pressure in the effective mass approximation and variational calculation scheme. The effect of applied hydrostatic pressure is introduced into the calculations using pressure dependent values of energy band gap and effective mass. Numerical results show that the ground-state shallow impurity binding energy E_b altered when both the hydrostatic pressure and *In* concentration increases for an on-center impurity. We have found that for large radii the binding energies are not affected by applied pressure. However, in the region where the particles interact with the barrier the binding energy is strongly dependent on the hydrostatic pressure for all x values. Furthermore, we have seen that the binding energy of the shallow impurity is affected more by the change of *In* concentration compared to the change of hydrostatic pressure.

Keywords: Quantum wires, Binding energy, Hydrostatic pressure, *In* concentration,

Sığ Safsızlık Bağlanma Enerjisinin Hidrostatik Basınç Altında *In* Konsantrasyonuna Bağlılığı

Özet

Çinko sülfür $In_xGa_{1-x}N/GaN$ silindirik kuantum telindeki (CQWWs) hidrojenik safsızlık taban durum bağlanma enerjisi, hidrostatik basınç altında *In* konsantrasyonu ve tel yarıçapının fonksiyonu olarak etkin kütle yaklaşımı ve varyasyonel teknikler kullanılarak incelendi. Uygulanan hidrostatik basınç etkisi, yasak enerji aralığı, tel yarıçapı ve etkin kütlenin basınca bağlılığı kullanılarak hesaplamalara katıldı. Hesaplamaların bağlanma enerjisi E_b' nin merkezdeki bir safsızlık için hem hidrostatik basınç hem de *In* konsantrasyonu arttırıldığında, bu parametrelere bağlı olarak değiştiğini gösterdi. Çok büyük tel yarıçaplarında bağlanma enerjisinin basınçtan etkilenmediği, Ancak parçacıkların engellerle etkileşmeye başladığı tel yarıçaplarında bağlanma enerjisi bütün x değerleri için hidrostatik basınca bağlı olduğu gözlendi. Ayrıca, *In* konsantrasyonunun ve hidrostatik basıncın bağlanma enerjisine etkisi karşılaştırıldığında *In* konsantrasyonundan kaynaklanan etkinin daha güçlü olduğu bulundu.

Anahtar Kelimeler: Kuantum teli, Bağlanma enerjisi, Hidrostatik basınç, *In* konsantrasyonu.

*Corresponding auther: Pınar Başer, pbaser@cumhuriyet.edu.tr.

Introduction

Recently, the wide-band gap group-III nitrides based on semiconductor heterostructures have attracted much attention due to their conspicuous device applications both in electronics and optoelectronics [1–3]. Group-III nitrides can be grown in two types: one of them is wurtzite crystal structure (WZ) and the other one is zinc-blende structure; these are produced in the thermodynamic stable configuration and in the metastable modification, respectively [4]. Due to its high crystal symmetry, spontaneous and the piezoelectric field in the ZB crystal structures are negligible, which makes them very useful for optoelectric device applications [5–8]. The binding energy of hydrogenic impurities in quantum well wires (QWWs) depends upon several micro-parameters such as material properties, impurity position and structural parameters. Also, some macro-parameters have significant effects on low dimensional systems such as external electric field, magnetic field, hydrostatic pressure and temperature. These macro-parameters are also widely studied; for example, Elabsy et al. have included the hydrostatic pressure effects to the Schrödinger equation and they have concluded that increasing external hydrostatic pressure gives rise to increased binding energy of donor impurities [9]. The effects of hydrostatic pressure on the binding energy and donor related photoionization cross-section in one dimensional (1D) and zero dimensional (OD) *GaAs* low dimensional systems have been performed by Correa et al. They have found that the photoionization cross-section increases with the applied hydrostatic pressure [10].

In this study, we used variational methods in the effective mass approximation scheme to calculate the binding energy of a shallow donor impurity in cylindrical $In_xGa_{1-x}N/GaN$ CQWWs under hydrostatic pressure for In concentration values x=0.2, 0.3 and 0.4 and on the center impurity at room temperature.

THEORY

The Hamiltonian for a hydrogenic donor impurity in the $In_xGa_{1-x}N/GaN$ CQWWs under the influence of hydrostatic pressure can be written as

$$H = H_0 - \frac{e^2}{\varepsilon|\mathbf{r}-\mathbf{r}_i|} \tag{1}$$

where $|\mathbf{r}-\mathbf{r}_i| = [\rho^2 + \rho_i^2 - 2\rho\rho_i\cos\phi + z^2]^{1/2}$ **r,** and $\mathbf{r_i}$ are the electron and impurity ion positions, respectively. For an impurity ion located at the wire axis, we take $\rho_i = 0$, which also simplifies the algebra. ε is the effective mean relative dielectric constant of the embedding material. Hamiltonian without Coulombic interaction H_0 can be written in cylindrical coordinates as

$$H_0 = -\frac{\hbar^2}{2m^*_{w,b}}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}+\frac{\partial^2}{\partial z^2}\right)+V(\rho,P) \tag{2}$$

where $m^*_{w,b}$ are the dependent effective masses in the well (w, $In_xGa_{1-x}N$) and barrier (b, *GaN*) regions The effective electron mass is given with $m^*_w = [0.19(1-x)+0.10x]m_0$ and $m^*_b = 0.19m_0$, where m_0 is the free electron mass[11].

$$m_{w,b}^{*}=\begin{cases} m_{w}^{*}, & \rho < R(P) \\ m_{b}^{*}, & \rho \geq R(P) \end{cases} \tag{3}$$

Similarly, the spatial pressure dependent confining potential $V(\rho,P)$ can be assumed as

$$V(\rho,P)=\begin{cases} 0, & \rho < R(P) \\ V_0(P), & \rho \geq R(P) \end{cases} \tag{4}$$

where the radius of the cylindrical wire is $R(P)$, and $V_0(P)$ is the conductor band offset. The pressure-dependent energy gap for ZB *GaN* and *InN* is given as follows [12],

$$\mathrm{E_g}(GaN)=3.22+(\gamma P+\delta P^2),\ \mathrm{E_g}(InN)=0.7+(\gamma P+\delta P^2) \tag{5}$$

A number of experimental [13,14] and theoretical [15-17] studies have investigated the band gap as a function of In content. The nonlinearity in the alloy band gap is conventionally expressed as

$$\mathrm{E_g}(Ga_{1-x}In_xN)=x\mathrm{E_g}(InN)+(1-x)\mathrm{E_g}(GaN)-bx(1-x) \tag{6}$$

where *b* is the *bowing parameter*. The band gap energy difference $\Delta \mathrm{E_g}$ can be writen as,

$$\Delta \mathrm{E_g}=E_g(GaN)-E_g(\mathrm{In_xGa_{1-x}N}) \tag{7}$$

and how $\Delta \mathrm{E_g}$ is distributed between the valance band ($\Delta \mathrm{E_v}$) and the conduction band ($\Delta \mathrm{E_c}$) offset. The band offset ($\Delta \mathrm{E_c}/\Delta \mathrm{E_v}$) is taken to be 70:30 following reference [18] . $\mathrm{V_0(P)}$ can be expressed as,

$$V_0(P)=\Delta \mathrm{E_g}(0.7) \tag{8}$$

The variation of wire radius $R(P)$ is given by [19]

$$R(P)=R_0*(1-(S_{11}+S_{12})*3P) \tag{9}$$

where S_{11} and S_{12} are the elastic compliance constants, which can be calculated using the definitions of elastic constants S_{11} and S_{12} given below [20].

$$S_{11}=\frac{C_{11}C_{33}-C_{13}^2}{(C_{11}-C_{12})(C_{33}(C_{11}+C_{12})-2C_{13}^2)} \tag{10}$$

$$S_{12} = \frac{C_{12}C_{33} - C_{13}^2}{(C_{11} - C_{12})(C_{33}(C_{11} + C_{12}) - 2C_{13}^2)} \tag{11}$$

The eigenfunctions of the Hamiltonian given with Eq (2) are

$$\psi_0(\rho, \phi, z) = Ne^{im\phi}e^{ik_z z}U(\rho), \qquad m = 0, \pm 1, \pm 2... \tag{12}$$

where N is normalization constant, k_z is the axial component of the electron's wave vector, $U(\rho)$ and $e^{im\phi}$ are the radial and angular parts of the electron wave function. $U(\rho)$ is given with linear combination of nth-order Bessel function J_n and modified Bessel function K_n. The radial part of wave function for the ground state $(m = 0,\ l = 1)$ is given by,

$$U(\rho) = \begin{cases} N J_0(r_{01}\rho) & , \quad 0 \le \rho \le R(P) \\ N \dfrac{J_0(r_{01}R(P))}{K_0(b_{01}R(P))} K_0(b_{01}\rho) & , \quad \rho > R(P) \end{cases} \tag{13}$$

Equation (13) satisfies the boundary conditions ($\rho = R(P)$)

$$\psi_{in}(\rho, \phi, z) = \psi_{out}(\rho, \phi, z)$$

$$\frac{1}{m_1^*(P)} \frac{\partial \psi_{in}(\rho, \phi, z)}{\partial \rho} = \frac{1}{m_2^*(P)} \frac{\partial \psi_{out}(\rho, \phi, z)}{\partial \rho} \tag{14}$$

while r_{01} and b_{01} are related with eigenvalue for the ground state E_0 of the problem in the absence of Coulomb term, inside and outside the wire, respectively. They are given as

$$E_0 = \frac{\hbar^2}{2m_1^*(P)}\left(r_{01}^2 + k_z^{\,2}\right) = \frac{\hbar^2}{2m_2^*(P)}\left(k_z^{\,2} - b_{01}^2\right) + V_0(P) \tag{15}$$

In order to obtain eigenvalues of Eq. 1, we need to include the impurity interaction. In this case an analytical solution cannot be obtained, so we use variational approach. We use the solution of equation (13) multiplied by a trial wave function chosen as $e^{-\lambda\sqrt{(\rho-\rho_i)^2+(z-z_i)^2}}$, where λ is a variational parameter, that is to be determined by minimizing the expectation value of the Hamiltonian in the presence of the Coulombic interaction [21]. Therefore, the trial wave function for the ground state with the impurity effect is given by,

$$\psi(\rho,z)=\begin{cases} N\,J_0(r_{01}\rho)e^{-\lambda\sqrt{(\rho-\rho_i)^2+(z-z_i)^2}} & ,\quad 0\le\rho\le R(P) \\ N\,\dfrac{J_0(r_{01}R(P))}{K_0(b_{01}R(P))}K_0(b_{01}\rho)e^{-\lambda\sqrt{(\rho-\rho_i)^2+(z-z_i)^2}} & ,\quad \rho>R(P) \end{cases} \tag{16}$$

The ground state electronic energy level E of the system with hydrogenic impurity can be obtained by minimizing the total energy,

$$E=\min_{\lambda}\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \tag{17}$$

Since we know now the energy values with and without the Coulombic interaction, the donor binding energy E_b can be defined as follows,

$$E_b(P)=E_0-E \tag{18}$$

For simplification, we transfer our variables to dimensionless ones with $\rho=tR$ variable change followed by scaling length and energy parameters using Bohr radius $a_B^*=\dfrac{\hbar^2\varepsilon}{m_b^*e^2}$ (for GaN $a_B=2.70\text{nm}$) and effective Rydberg $R_B^*=\dfrac{m_b^*e^4}{2\hbar^2\varepsilon^2}$, (for GaN $R_B=27.48\text{meV}$) for P=0, respectively. After some algebra parallel to no pressure case [22], hydrogenic impurity binding energy as a function of λ, is given with

$$\widetilde{E}_b(R(P),P)=-(\lambda a_B)^2\frac{(d/d\lambda)\left(I_1+\dfrac{m_1^*}{m_2^*}I_2\right)}{(d/d\lambda)(I_1+I_2)}-4a_B\frac{[I_1+I_2]}{\dfrac{\partial}{\partial\lambda}[I_1+I_2]} \tag{19}$$

where I_1 and I_2 represent integrals that needed to be calculated numerically and their explicit forms are given below in dimensionless variables.

$$I_1=R^2(P)\int_0^1 t\,J_0^2(r_{01}tR)K_0(2\lambda R(P)t)dt \tag{20}$$

$$I_2=R^2(P)\frac{J_0^2(r_{01}R(P))}{K_0^2(b_{01}R(P))}\int_1^{\infty} t\,K_0^2(b_{01}tR)K_0(2\lambda R(P)t)dt \tag{21}$$

Equation (19) can be numerically solved for a specific λ value that minimizes it for any given *R(P)* values.

Results and Discussion

We have calculated the shallow impurity binding energy $E_b(P)$ as a functions of the hydrostatic pressure for shallow impurity placed in the center of CQWWs. Parameters, such as potential height $V_0(P)$, wire radius $R(P)$ and In content x used in calculations are taken from Ref. [23].

In Fig.1-a, b and c the shallow impurity binding energy $E_b(P)$ is investigated as a function of wire radius for different external hydrostatic pressures P=0, 10 and 20 GPa, respectively. In our calculations x is taken as 0.2, 0.3 and 0.4. In fig. 1-a, it is seen that the shallow impurity binding energy maximizes at the following radii: 10.82, 7.84 and 7.03 Å for x=0.2, 0.3 and 0.4, respectively. In fig. 1-b, the shallow impurity binding energy maximizes at the following radii: 9.44, 7.34 and 6.92 Å for x=0.2, 0.3 and 0.4, respectively and similarly, in fig. 1-c shallow impurity binding energy maximizes at the following radii: 8.96, 7.31 and 6.72 Å for x=0.2, 0.3 and 0.4, respectively. The maximum value of the shallow impurity binding energies slightly move to the narrow wire widths as the pressure and *In* concentration increases because the effective Bohr radius of the impurity state decreases with pressure and *In* concentration.

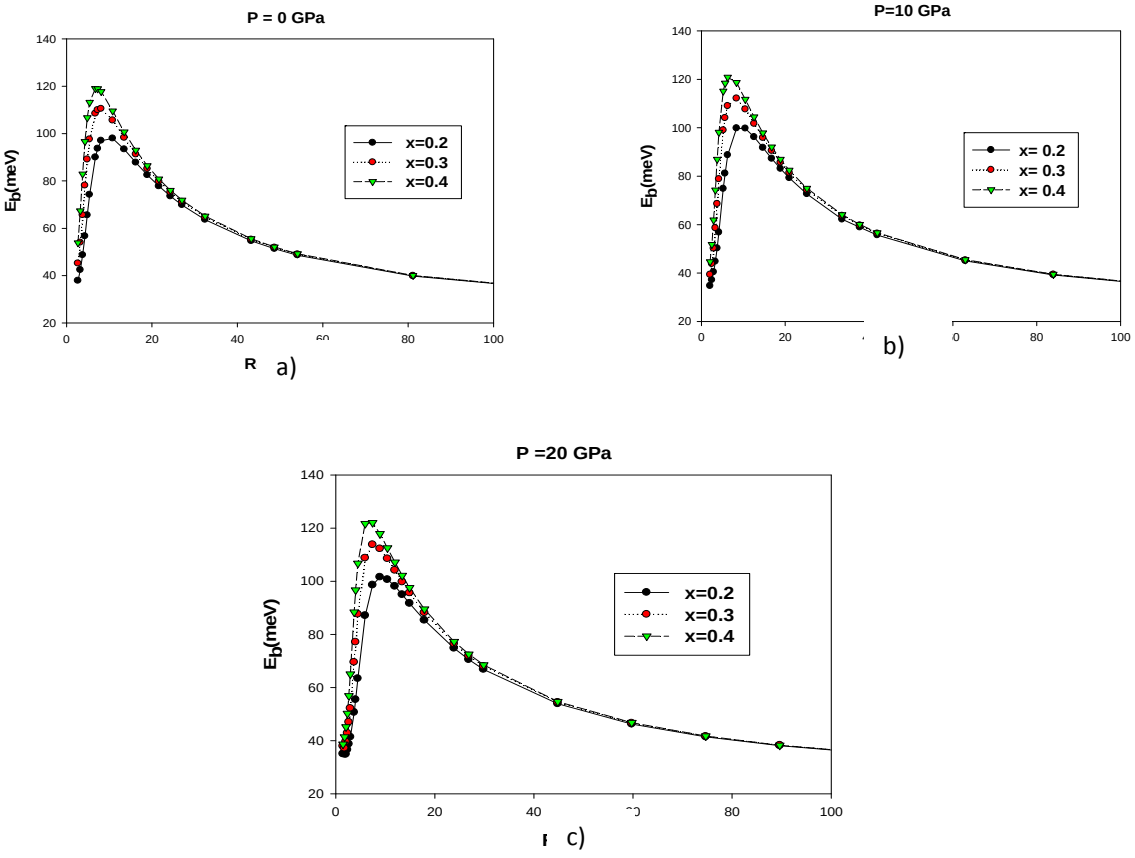

Fig. 1. Ground-state shallow impurity binding energy as a function of the wire radius of ZB $In_xGa_{1-x}N/GaN$ (x=0.2, 0.3 and 0.4) quantum wire for external pressure a) P=0 GPa, b) P=10 GPa c) P=20 GPa for on-center impurity.

In Fig.1, it is also seen that for large wire radii the particle sees no spatial confinement effects so the binding energies converge to bulk $In_xGa_{1-x}N$ ground state binding energy values. As wire radius gets smaller, the binding energy increases since the spatial confinement gets stronger. That is, the distance between the electron and the impurity is decreased when the wire radius *R(P)* is decreased, which makes the binding stronger. Further decreasing the wire radius maximizes the binding energy to the quantum confinement limits then it drops rather sharply to the characteristic bulk value of the barrier material *GaN* in all cases. This is due to the fact that as the spatial confinement forces to localize particle in a smaller space then the quantum confinement effects kicks in, that is, particles cannot be localized further due to uncertainty principle and they start leaking out to the barrier reducing the binding energy sharply.

Furthermore, we have seen that effect of the binding energy of the In concentration are very influential than the hydrostatic pressure. This influence has been showed in Table.1

Table 1: To illustrate the binding energy dependency to hydrostatic pressure and *In* concentration, we have tabulated the binding energy maxima positions.

x / P(GPa)	0.2	0.3	0.4
0	97.96	110.47	119.00
10	99.79	112.11	120.85
20	101.54	113.72	121.99

In Table1, it shows that the binding energy depends on both hydrostatic pressure and In concentration. If the hydrostatic pressure is increased from 0 GPa to 20 GPa, the impurity binding energy change from 97.96 meV to 101.54 meV for x=0.2. This increase is about %3.65. On the other hand, we increase In concentration from 0.2 to 0.4 for P=0 GPa, binding energy increase from 97.96 meV to 119.00 meV. This increase is about %21.47. If we compare with variation of the case for *GaAs* based material, effect of the hydrostatic pressure of structure in this study is around % 3.65 for x=0.2. However, this effect is around 42% in $GaAs/ Ga_{1-x}Al_xAs$ CQWWs for the same wire width [24].

In Fig. 2, barrier height is calculated as a function of the hydrostatic pressure in the ZB $In_{0.2}Ga_{0.8}N/GaN$ CQWWs for different In concentration x=0.2, 0.3 and 0.4.

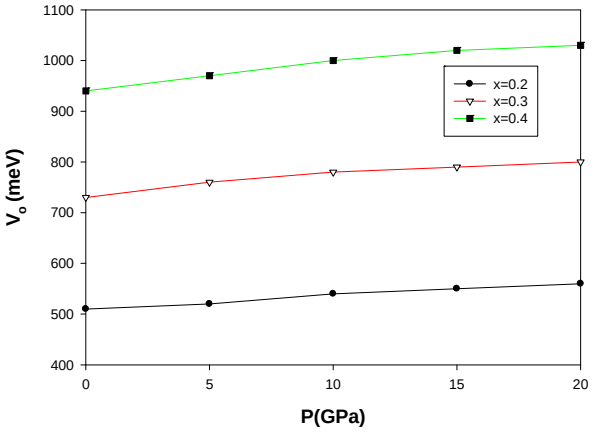

Fig. 2. The height of barrier as a function of the pressure of ZB $In_{0.2}Ga_{0.8}N/GaN$ quantum wire for x=0.2, 0.3 and 0.4.

In Figure 2, it is shown that height of barrier increases as the hydrostatic pressure P increases. This is because the band gap of ZB $In_xGa_{1-x}N$ material is decreased when the hydrostatic pressure P increased, which relatively raises the height of the barrier and enhances the confinement of impurity states resulting a higher binding energy. However, this increase in binding energy is not uniform everywhere. It is stronger for mid range wire radius values and almost diminishes for larger or very small wire radii. This is due to the fact that for very large wire radii the particle is far away from the barriers; therefore, it does not sense how high the barrier is. In the other extreme, the wire radius is so small that the particle cannot reside in the well, so it leaks out totally to the barrier.

In Figure 3, the ground-state impurity binding energy is calculated as a function of the hydrostatic pressure using the different wire radius as a parameter for an on-center impurity at x=0.4.

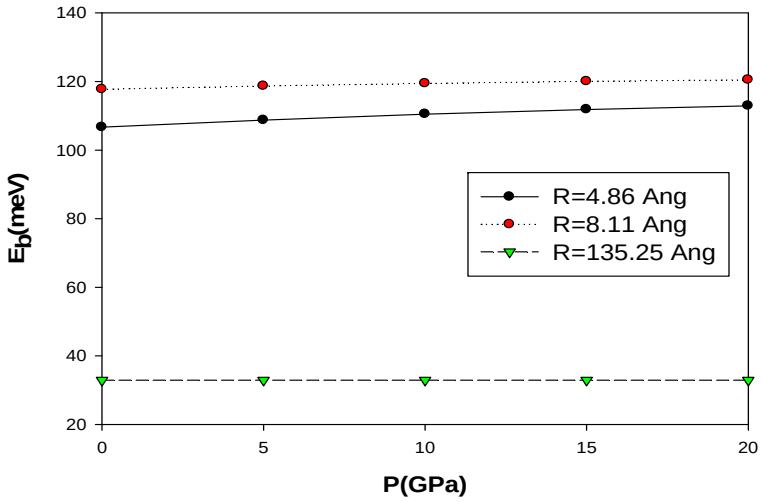

Fig. 3: The ground-state donor binding energy of an on-center impurity as a function of external pressure for different values of the wire radius in ZB $In_{0.4}Ga_{0.6}N/GaN$ quantum wires structure.

It is shown that the ground-state binding energy increases except for in the large wire radii as hydrostatic pressure P increases. It is seen that the ground state binding energy increases with

the pressure since the quantum well radius decreases with increasing pressure, so the distance between charged particles decreases when the binding energy increases.

Conclusion

We have calculated the ground state binding energy of hydrogenic impurity in ZB $In_xGa_{1-x}N/GaN$ CQWWs under hydrostatic pressure using variational procedures within the effective mass approximation. In calculations, the pressure dependency of the effective mass, well radius and potential height are taken into account. The results show that the donor binding energy increases with the increasing pressure and *In* concentration x. However, this increase in binding energy is not uniform everywhere. Furthermore, we have seen that effect of the binding energy of the *In* concentration are more influential than the hydrostatic pressure. Also, the binding energies close to binding energy maxima are dependent both to In concentration and hydrostatic pressure. As a result, it can be said that the effect of In concentration x is only noticeable for radii nearby binding energy maxima. Finally, even though the pressure dependency seems much weaker than $GaAs/Ga_{1-x}Al_xAs$ based CQWWs, we still have enough room to tune the binding energy values via external hydrostatic pressure.

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