Cumhuriyet Science Journal
e-ISSN: 2587-246X
ISSN: 2587-2680
Cumhuriyet Sci. J., 41(3) (2020) 699-705
http://dx.doi.org/10.17776/csj.747296

Pressure and temperature effects on magnetoelectric band energies in GaAs / $In_xGa_{1-x}As$ cylindrical quantum wires

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Abstract

Low-dimensional systems, consisting of GaAs / InGaAs heterostructures, have attracted considerable attention due to their many applications in optoelectronic and microelectronic devices. In the present work, the electron and the heavy-hole ground state energy in an InGaAs/GaAs cylindrical quantum well wires (CQWWs) is investigated with the consideration of geometrical confinement. The ground state energy was calculated as a function of hydrostatic pressure and temperature. Under the constant pressure and at a certain magnetic field value, while the ground state energy of the electron and the hole decreases depending on the temperature, it is observed that the energy increases as the hydrostatic pressure increases under the constant temperature. These calculations are interpreted with graphics.

Article info

History:
Received: 02.06.2020
Accepted: 05.08.2020
Keywords:
Ground State Energy, GaAs/ $In_xGa_{1-x}As$ Quantum Wire, Hydrostatic Pressure, Temperature

1. Introduction

Heterostructures are semiconductor devices obtained by the development of crystal growth techniques. It is used in the construction of high performance, fast and high frequency optical devices with heterostructures. Particle movements can be controlled in these structures, thus providing a high advantage in device designs. Low-dimensional structures include quantum wells (QWs), quantum well wires (QWWs) and quantum dots (QDs)[1-3].

As the III-V group semiconductors InAs is active in the infrared region, it has found wide application in optoelectronic systems. For some applications there is a need of good quality InAs layers. The electron mobility of the InAs semiconductor compound is equal to 30000 cm^2/Vs and is approximately three times greater than the mobility value of the GaAs semiconductor material.The mobility is proportional to the carrier conductivity. As mobility increases, so does the current-carrying capacity of transistors. A higher mobility shortens the response time of photodedectors. A larger mobility reduces series resistance, and this improves device efficiency and reduces noise and power consumption. The band gap value of the InAs semiconductor compound is 0.35 eV and is four times smaller than that for GaAs. This makes InAs / InGaAs compound based devices exhibit good electronic performance [4-6].

Alloys such as $In_xGa_{1-x}As$ are used in detector structures, especially in semiconductor technology. In gallium indium arsenic (InGaAs), there is contact of indium semiconductor compound to gallium arsenic. Generally, it can be used in high power, high frequency electronics and it is superior to other known semiconductors such as silicon and gallium arsenic (GaAs) due to the high speed movement of the electron in this material group and the femtosecond life span of the carriers. The band spacing of indium gallium arsenic (InGaAs) has made this material indispensable for the construction of the detector, especially for fiber optic communications around 1300 and 1500 nm [7- 8]. InGaAs was first obtained in 1978 by T. P. Pearsall by growing it on indium phosphate (InP) [9]. Pearsall found the bandwidth of this material, the effective mass of electrons and holehalls, their mobility and the properties of $In_xGa_{1-x}As$.

High Electron Moblity Transistor (HEMT) devices made using $In_xGa_{1-x}As$ are one of the fastest transistor types, and this material is a

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very popular material for infrared detectors. $In_xGa_{1-x}As$ has become more preferable (replaced by Germanium) due to the high stability current of germanium used in these materials. It is generally used in short wavelength infrared cameras. It can also be used to produce $In_xGa_{1-x}As$ laser. Lasers of 905nm, 980nm, 1060nm and 1300nm were produced [10-12].

Hydrostatic pressure and temperature is a preventive external parameter that changes the electronic and optical properties of devices made of semiconductor materials. Therefore, the dependence of the optical and electrical properties of the GaAs / GaAlAs and GaAs/ InGaAs systems under pressure, temperature, electric and magnetic fields has attracted considerable attention [13-15].

In this study, the variation of electron and hole ground state energy levels in the cylindrical quantum well wire (CQWW) with GaAs / $In_xGa_{1-x}As$ was calculated with temperature and pressure. Numerical results showed that the particle ground state energy in QWs is highly dependent on external parameters.

2. Theory

Using the Hamiltonian new effective mass approach of the electrons and heavy-hole particles in GaAs/ $In_xGa_{1-x}As$ CQWWs, the temperature can be written as below, under hydrostatic pressure, and outside magnetic field [16].

$$H=\frac{1}{2m_e^*(P,T)}\left(\vec{P}_e+\frac{e}{c}\vec{A}_e\right)^2+\frac{1}{2m_h^*(P,T)}\left(\vec{P}_h-\frac{e}{c}\vec{A}_h\right)^2+V_e(\rho_e,P,T)+V_h(\rho_h,P,T) \qquad (1)$$

where $\vec{P}_{e(h)}$ is the momentum operator, $\vec{A}_{e(h)}$ is the vector potential of the magnetic field, which is written as $\vec{A}(\vec{r})=\frac{1}{2}(\vec{B}\times\vec{r})$, with $\vec{B}=B\hat{z}$. In cylindrical coordinates, the components of the vector potential are chosen as $A_\rho=A_z=0$ and $A_{\phi\, e(h)}=\frac{B\rho_{e(h)}}{2}$. The subscripts e and h stand for electron and hole, respectively. $m_{e(h)}^*(P,T)$, $\varepsilon(P,T)$ and $V_{e(h)}\left(\rho_{e(h)},P,T\right)$ are hydrostatic pressure and temperature dependent effective masses, dielectric constants and spatial confinement potentials. Since the effective masses of GaAs and $In_xGa_{1-x}As$ are close together, the effective mass of GaAs is used in calculations [17]. Dependence of the electron active mass on the hydrostatic pressure and temperature is given by Eq. 2 [23].

$$m_e^*(P,T)=\left[1+E_P^\Gamma\left(\frac{2}{E_g^\Gamma(P,T)}+\frac{1}{E_g^\Gamma(P,T)+0.341}\right)\right]^{-1}m_0 \qquad (2)$$

For heavy hole the temperature dependency is ignored and hydrostatic pressure dependency is given by

$$m_h^*(P)=[0.134+(a_2P+a_3P^2)]m_o \qquad (3)$$

where $a_2=-0.1\times10^{-2}$ GPa^{-1} and $a_3=5.5\times10^{-4}$ GPa^{-2}. The isotropic hole mass is defined in Eq 3. In calculation, the values of the physical parameters pertaining to the material GaAs in Ref [23] is used the heavy hole isotropic hole mass is calculated from

$$(m_h^*)^{-1}=\left(\frac{2}{3}\right)(m_h^*(x,y))^{-1}+\left(\frac{1}{3}\right)(m_h^*(z))^{-1} \qquad (4)$$

It was used as in $\varepsilon(P,T)$ is the pressure and temperature dependent static dielectric constant and given by [18-20].

$$\varepsilon(P,T)=\begin{cases}12.74\,e^{-1.67*10^{-2}P}\,e^{9.4*10^{-5}(T-75.6)}, & T\le 200K\\ 13.18\,e^{-1.73*10^{-2}P}\,e^{20.4*10^{-5}(T-300)}, & T>200K\end{cases} \qquad (5)$$

Similarly, $E_g^\Gamma(P,T)$ is the band gap defined for GaAs and InGaAs semiconductors.

$$E_g^\Gamma(P,T)=E_g^0+\alpha P-\beta T^2(T+c)^{-1} \qquad (6)$$

For the parameter values in this equation, Ref. [17] can be seen. The confinement potential $V_{e(h)}(\rho_{e(h)},P,T)$ is given by

$$V_{e(h)}\left(\rho_{e(h)},P,T\right)=\begin{cases}V_{0e(h)}(P,T) & \rho_{e(h)}\ge R(P)\\ 0, & \rho_{e(h)}<R(P)\end{cases} \quad [22] \qquad (7)$$

$\rho_{e(h)}$ is the spatial confinement variable in cylindrical coordinates for electron and hole. Where $V_{0e}(P,T)$ and $V_{0h}(P,T)$ are the confinement potentials of the electron and hole, respectively and the values of $V_{0e}(P,T)$ and $V_{0h}(P,T)$ can be defined as in Eq. 8 [21].

$$V_{0e}(P,T) = G_c\left(E_g^{GaAs}(P,T) - E_g^{GaInAs}(P,T)\right)$$
$$V_{0h}(P,T) = G_v\left(E_g^{GaAs}(P,T) - E_g^{GaInAs}(P,T)\right) \quad (8)$$

where G_c and G_v are conductivity band offset and valence band offsets respectively, in this study the values are taken as 0.7 and 0.3. R (P) is defined as the pressure radius of the well as in Eq. 9,

$$R(P) = R(0)[1 - 3\mathrm{P}(S_{11} + 2S_{12})P]^{1/2} \quad (9)$$

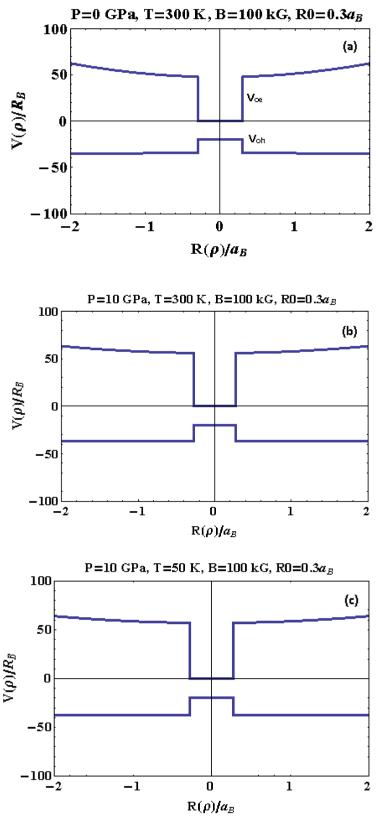

Figure 1: Spatial and parabolic confinement for B = 100 kG **a)** P=0 kG, T=300 K **b)** P=10 kG, T=300 K, **c)** P=10 kG, T=50 K.

Where $R(0)$ is the wire radius without hydrostatic pressure and S_{11} and S_{12} are the compliance constants of GaAs [22, 23]. In Figure 1, the potential profile consisting of the sum of the parabolic siege and the spatial siege originating from the magnetic field is given with the press and temperature.

The ground state wave function in CQWWs under magnetic field, hydrostatic pressure and temperature [24]. The wave functions for the electron and hole ground state are given by Eq. 10.

In Eq. 10 the variable N is the normalization constant, ${}_1F_1(-a_{01},1,\xi)$ and $U(-a'_{01},1,\xi)$ are confluent hypergeometric functions which are corresponding solutions of inside and outside of the CQWWs respectively, in the presence of a uniform magnetic field parallel to the wire axis. We defined the variable $\xi_{e(h)} = \frac{\rho_{e(h)}^2}{2\alpha_{c[e(h)]}^2}$ in terms of cyclotron radius $\alpha_{c[e(h)]} = \sqrt{\frac{\hbar}{m_{e(h)}^*\omega_{c[e(h)]}}}$ where $\omega_{c[e(h)]} = \frac{eB}{m_{e(h)}^*}$ is the cyclotron frequency. The Eq. 10 satisfies the boundary condition $\frac{\partial\psi_{int}}{\partial\rho_{e(h)}} = \frac{\partial\psi_{ext}}{\partial\rho_{e(h)}}$ at, $\rho_{e(h)} = R(P)$, the normalization constant (N), $a_{01e(h)}$ and $a'_{01e(h)}$ are the eigenvalues for the ground state of the problem inside and outside the wire for an electron and hole, respectively. E_{e1} and E_{hh1} are magnetoelectric band energies for the lowest energy electron and highest energy heavy hole in the conductivity band and valence band. Ref. [24] terminology is calculated and the ground state of the system, electron (E_{e1}) and hole energy (E_{hh1}), respectively are found as follows.

$$E_{e1} = \hbar\omega_{c(e)}\left(a_{01(e)} + \frac{1}{2}\right)$$
$$E_{hh1} = \hbar\omega_{c(h)}\left(a_{01(h)} + \frac{1}{2}\right) \quad (11)$$

$$\psi(\overrightarrow{\rho_e},\overrightarrow{\rho_h}) = \begin{cases} N\exp\left(-\frac{\xi_e}{2}\right)\ {}_1F_1(-a_{o1(e)},1,\xi_e), & \rho_e \le R(P) \\ N\frac{{}_1F_1(-a_{o1(e)},\ 1,\ \xi_{R(e)})}{U\left(-a'_{o1(e)},\ 1,\xi_{R(e)}\right)}\exp\left(-\frac{\xi_e}{2}\right)U\left(-a'_{o1(e)},1,\xi_e\right), & \rho_e > R(P) \\ N\exp\left(-\frac{\xi_h}{2}\right)\ {}_1F_1(-a_{o1(h)},1,\xi_h), & \rho_h \le R(P) \\ N\frac{{}_1F_1(-a_{o1(h)},\ 1,\ \xi_{R(h)})}{U\left(-a'_{o1(h)},\ 1,\xi_{R(h)}\right)}\exp\left(-\frac{\xi_h}{2}\right)U\left(-a'_{o1(h)},1,\xi_h\right), & \rho_h > R(P) \end{cases} \quad (10)$$

3. Results and Discussion

We chose semiconductor parameters to avoid complications. For example, the compound $In_{0.53}Ga_{0.47}As$ is known to transform when the Ga alloy concentration goes beyond x = 0.6 [gamma-L transition] and x = 0.8 [gamma-x transition. Therefore, the In concentration was chosen as x = 0.47 [25]. Also in calculations, effective mass values of GaAs were taken as $m_e^* = 0.067m_o$ and $m_h^* = 0.135m_o$. For InGaAs / GaAs semiconductor compound, Rydberg Constant $R_B = m_e^* e^4/2\hbar^2\epsilon^2 \sim 5.80meV$ and Bohr Radius $a_B = \hbar^2\varepsilon/m_e^*\ e^2\ \sim(94.53\dot{A})$ are equal to, where $\varepsilon = 13.13$ is the dielectric constant for GaAs.

Fig. 2 shows the change of electron and hole ground state energy with hydrostatic pressure. In these calculations, wire radius R = 0.3a_B, T = 300 K and B = 100 kG were used.

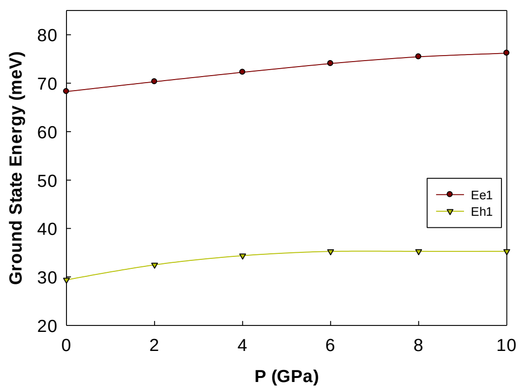

Figure 2: Ground state electron and heavy- hole ($E_{e(hh1)}$) energy as a function of hydrostatic pressure for R = 0.3 a_B, T = 300 K and B = 100 kG.

Fig. 3 shows the variation of electron and heavy hole ground state energy with temperature (T) for In concentration x = 0.47 at P = 0 GPa and B = 100 kG.

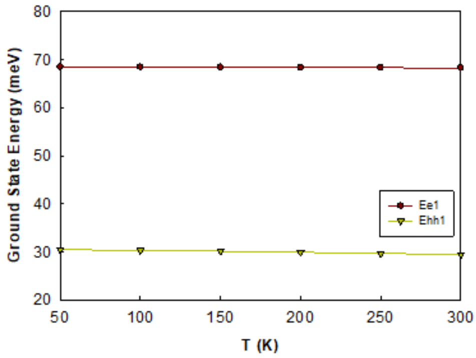

Figure 3. Ground state electron and hole energy ($E_{e(hh1)}$) as a function of temperature for R = 0.3 a_B, T = 300 K and B = 100 kG

When Table 2 is examined, when the temperature is changed between 0-300 K, it is seen that the biggest change in the parameters in the table occurs in the value of the dielectric constant, and even this change is about 2%. Changes in other parameters are much smaller than this value. For example, when the temperature for the electron is 50 K, E_{e1} = 68.52 meV. When the temperature was increased to 300 K, it was calculated as E_{e1} = 68.28 meV. The amount of change between these values is less than 0.3%.

It is clear from Table 2 that the dependence of the ground state energy in the GaAs/ InGaAs system on temperature is negligible, that is, the system is very stable under temperature changes. On the other hand, hydrostatic pressure appears to be very effective when the parameter changes in Table 1 are examined on the system. The potential height and the effective mass increase with increasing pressure, thereby increasing the energy.

Table 1. The variation of dielectric constant, effective masses, potential heights and wire radius, with hydrostatic pressures for T = 300 K and B=100 kG.

P(GPa)	€ (P, T)	m_e/m_0	m_h/m_0	V_{0e}(meV)	V_{0h}(meV)	R/a_B
0	13.18	0.063	0.146	476.2	204.2	1.00
2	12.73	0.072	0.148	508.8	217.7	0.98
4	12.29	0.080	0.151	531.8	227.9	0.97
6	11.88	0.087	0.16	547.9	234.8	0.95
8	11.47	0.092	0.173	556.3	238.4	0.94
10	11.08	0.096	0.191	556.97	238.7	0.92

Table 2. The variation of dielectric constant, effective masses, potential heights and wire radius, with temperatures for P=0 GPa and B=100 kG.

T(K)	€ (P, T)	m_b/m_0	m_w/m_0	V_{0e}(meV)	V_{0h}(meV)
0	13.52	0.066	0.0416	487.5	208.9
50	12.70	0.066	0.0415	486.7	208.5
100	13.58	0.066	0.0411	485.1	207.9
150	13.61	0.065	0.0407	481.1	206.1
200	13.66	0.064	0.0402	481.0	206.0
250	13.73	0.064	0.0396	478.7	205.2
300	13.80	0.063	0.0389	476.5	204.2

4. Conclusion

We calculated the magneto electric band energies for electron and heavy hole particles under R = 3a_B and B = 100 kG magnetic field as a function of hydrostatic pressure and temperature using the effective mass approach in a one-dimensional GaAs / InGaAs cylindrical quantum well wires. The graphs show that as the hydrostatic pressure increases in both particles, the ground state energy increases. This increase in pressure and energy can be explained by looking at the value of the parameters. As pressure increases, wire radious and dielectric constant decrease while the confinement potential and effective mass value increase. In this case, particle energies increase as the quantum confinement effects on the electron and hole increase.

The effective mass and potential height decrease as the dielectric constant increases with temperature. We can say that the temperature change almost does not affect the electronic energy and the hole energy because when the Table 2 is examined, it is seen that the amount of change of the parameters is less than 2%. As it is clearly seen in Fig. 1 b) and c), at P = 10 GPa, at T = 50 K and T = 300 K, a small amount of decrease is observed as the temperature rises. However, increasing dielectric constant and decreasing potential height reduces the confinement effects of the particle and contributes to the reduction of electronic energy as the reduction in effective mass increases the mobility of the particle. Furthermore, we have also shown that, the binding energy is very stable for a large (0-300K) of temperature variation.

Conflicts of interest

The author state that did not have conflict of interests.

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