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Photo-ionization Cross-Section and Binding Energy of Exciton in a Parabolic Quantum Well

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Abstract - *Parabolic quantum well has attracted considerable attention of the researchers because of its applications such as speed circuits, optical devices etc. Binding energies of ground and excited states of heavy hole exciton and light hole exciton in a parabolic quantum well composed of* $GaAs/Ga_{1-x}Al_xAs$ *with potential profile proportional to* $\left|\frac{z}{L/2}\right|^2$ *have been calculated as a function of wellwidth (L) and Al concentration (x). The photo-ionization cross-section of exciton has been calculated as the function of photon energy* $(\hbar\omega)$ *and wellwidth (L) by variational method. The results show that the binding energy decreases with increased wellwidth of the quantum well but increases with Al concentration. The photo-ionization cross-section decreases with increased photon energy but increases as wellwidth increases. The photo-ionization cross section is a useful tool to detect positions of charge carriers inside the quantum structures.*

Key Words: Exciton, Binding energy, Photo-ionization cross-section, Parabolic quantum well

1. INTRODUCTION

There has been tremendous interest in the study of structural, electronic and optical properties of low dimensional structures during past few years due to its potential applications in opto-electronic device fabrication. It is possible to fabricate the nanostructures such as quantum wells, quantum wires and quantum dots with various potential profiles like Rectangular, Triangular, Near Triangular and surface using the advanced epitaxial growth techniques such as molecular beam epitaxy (MBE) and metal organic chemical vapour deposition (MOCVD).

The Quantum wells with parabolic profile (Parabolic quantum well - PQW) have been studied by several researchers. Yuan Lihua et al have studied the binding energies of the ground state and excited state of a hydrogenic donor in the ZnO parabolic quantum well [1].

Meshad et al [2] have showed the binding energy of a neutral donor in GaAs-Al_x $Ga_{1-x}As$ parabolic quantum well is determined variationally, the changes in the binding energy of donors are calculated, for different well sizes and depths. Wang et al [3] have calculated the ground and first excited-state binding energies of a hydrogenic donor in a rectangular quantum dot (RQD) in the presence of electric field. M. Arulmozhi [4] have calculated donor binding energies in nano-quantum wells with parabolic confinement and the result shows that binding energy of donor increases when the external pressure increases and the binding energy decreases when the temperature increases.

E.C.Niculescu [5] have calculated the effective mass approximation for the states of single and double donors in a finite parabolic quantum well is presented. The validity of the infinite-parabolic-well approximation is also discussed. Alvarado-Reyes et al [6] have investigated the binding energy of impurity as a function of the impurity position and wellwidth within the effective mass approximation using a variational approach. The results show that an inverse parabolic quantum well turns into a parabolic quantum well with the effect of the magnetic field. El-Meshand et al [7] have calculated the binding energy of an exciton bound to the quantum well structure is then determined using a standard variational technique. Arulmozhi et al [8] have calculated the binding energy of near triangular quantum well (NTQW) in magnetic field and also calculated the binding energy of exciton in $ZnSe/Zn_{1-x}Mg_xSe$ quantum well with Poschl-teller Potential [9].

El-Meshad et.al [10] have solved variationally the binding energy of a neutral donor in $GaAsAl_x/Ga_{1-x}As$ parabolic quantum well, the changes in the binding energy of donors are calculated for different well sizes and depths. El-said et.al [11] have calculated the photo-ionization cross-section on photon energy for shallow donors in a finite barrier $GaAs/Ga_{1-x}AsAl_x$ quantum wells as the binding energy as a function of well width. One of important approximations have been made in this work is to take the second subband states as the final state in the photo-ionization process, because the photo-ionization cross-section approximations

have been depend on the ground and first excited states. Ilaiwi et.al [12]have calculated the photo-ionization cross-section on photon energy for shallow donors in a finite barrier GaAs/$Ga_{1-x}AsAl_x$ quantum wells as the binding energy as a function of well width. The effect of a magnetic field is also considered. Sali et.al [13] have calculated the photon energy dependence of the photo-ionization cross section for a hydrogenic donor impurity in an infinite barrier GaAs quantum dot as a function of the sizes of the dot and the impurity position. The measurements of the photo-ionization in such systems would be of great interest in understanding the optical properties of carriers in quantum dots.

Kasapoglu et.al [14] have calculated the hydrostatic pressure and electric field effects on the donor impurity related photo-ionization cross-section and impurity binding energy in GaAs/GaAlAs quantum well-wires. C.E.Niculescu [15] have studied the binding energy and photo-ionization cross-section of a donor impurity in a pyramid shaped quantum dot under simultaneous action of a hydrostatic pressure and high-frequency laser field. Kasapoglu et.al [16] have calculated the impurity position dependence of the photo-ionization cross-section and the binding energy for a hydrogenic donor impurity in a quantum well wire in the presence of the electric and magnetic field as a function of the photon energy. Jayam et.al [17] have investigated the photo-ionization of impurities in quantum well systems.

In this paper, the photo-ionization cross-section of exciton in a parabolic quantum well composed of GaAs/$Ga_{1-x}Al_xAs$ has been calculated as the function of photon energy $(\hbar\omega)$ and wellwidth (L) by variational method. The binding energies of ground and excited states of heavy hole exciton and light hole exciton has been investigated as a function of wellwidth (L) and Al concentration(x). Finally these reports are compared with available literature.

2. THEORY

2.1 Binding Energy of Exciton for Ground and Excited States

The Hamiltonian of an exciton in PQW in effective mass approximation is given by [18],

$$H = -\frac{\hbar^2}{2\mu_{hi}^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right]-\frac{\hbar^2}{2m_e^*}\frac{\partial^2}{\partial z_e^2}-\frac{\hbar^2}{2m_{hi}^*}\frac{\partial^2}{\partial z_h^2}-\frac{e^2}{\varepsilon_o|r_e-r_h|}+V_e(Z_e)+V_h(Z_h) \quad (1)$$

$$H = -\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right]-\frac{\mu_{hi}^*}{m_e^*}\frac{\partial^2}{\partial z_e^2}-\frac{\mu_{hi}^*}{m_{hi}^*}\frac{\partial^2}{\partial z_h^2}-\frac{2}{|r_e-r_h|}+V_e(Z_e)+V_h(Z_h) \quad (2)$$

where ħ is the plank's constant(1.05459×10^{-27}), m_e^* is the effective mass of electron, m_{hi}^* is the effective mass of hole, if there is i=h heavy hole $(m_{hh}^*=0.34m_o)$ or if there is i=l light hole $(m_{lh}^*=0.094m_o)$, ε_o dielectric constant, e (4.08324×10^{-10}) is the charge of electron and r is given by

$$r=\sqrt{\rho^2+|Z_e-Z_h|^2}.$$

If i=h μ_{hh}^* is the reduced mass of heavy hole or if i=l μ_{lh}^* is the reduced mass of light hole

$$\frac{1}{\mu_{hi}^*}=\frac{1}{m_e}+\frac{1}{m_{hi}}$$

where equation (1) is SI units, equation (1) is converted to Rydberg units in the form of equation (2) therefore we have used the effective Rydberg as the unit of energy $R^*=\frac{\mu_{hi}^*e^4}{2\hbar^2\varepsilon_o^2}$ for the exciton. The unit of length is the effective Bohr radius $a^*=\frac{\hbar^2\varepsilon_o}{\mu^*e^2}$ for the exciton.

The potential profiles for the electron and the hole in parabolic potential well [7] are given by

$$V(z)=\begin{cases}V_o\left|\frac{z}{\frac{L}{2}}\right|^2 & |Z|<\frac{L}{2}\\ V_o & |Z|<\frac{L}{2}\end{cases} \quad (3)$$

where, V_o is the barrier height, which depends on the composition x of Al and Z=Z_e (electron) or Z_h (hole).

We apply the variational approach to solve the nonlinear Schrödinger equation (2). The trial wavefunction for the ground state is given by [1, 5, 18 and 19],

$$\psi_i(z_e, z_h, r) = \begin{cases} A\, e^{-\alpha_e^2 z_e^2}\, e^{-\alpha_h^2 z_h^2}\, e^{-ar} & |z| < \frac{L}{2} \\ B\, e^{-\beta_e z_e}\, e^{-\beta_h z_h}\, e^{-ar} & |z| > \frac{L}{2} \end{cases} \quad (4)$$

And the trial wavefunction for the first excited state is given by,

$$\psi_f(z_e, z_h, r) = \begin{cases} A\,\rho\, e^{-\alpha_e^2 z_e^2}\, e^{-\alpha_h^2 z_h^2}\, e^{-ar} & |z| < \frac{L}{2} \\ B\,\rho\, e^{-\beta_e z_e}\, e^{-\beta_h z_h}\, e^{-ar} & |z| > \frac{L}{2} \end{cases} \quad (5)$$

where $z_e, z_h = \frac{L}{2}$, a is the variational parameter and A and B are the normalization constant.
α, β are the constants given by

- $\alpha_i = \left(\frac{v_{oi}}{L^2}\right)^{\frac{1}{4}}$ in effective Rydbergs and effective Bohr radius.
- $\beta_i = \sqrt{(v_{oi} - E_i)}$ in effective Rydbergs and effective Bohr radius.

According to Bohr-Somerfield quantization rule E_i can be written as,

- $E_i = \frac{2\hbar}{R^* a^* L}\left(\frac{2R^* v_o}{m_i^*}\right)^{\frac{1}{2}}\left(n - \frac{1}{2}\right)$ in effective Rydbergs and effective Bohr radius.

where $\hbar$ the Planck 's constant, L is the wellwidth in nanometer, v_o is the barrier height, m_i^* effective mass, n is denoted as quantum states, E_i is the energy of the states if $i = e$ is the barewell energy of electron and the $i = h$ is the barewell energies for heavy and light hole.

The energies of the ground state and first exited state are determined by minimizing the expectation value of the Hamiltonian:

$$< H >= \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \quad (6)$$

Using these Hamiltonian in equations (1) and (2) and the appropriate trial functions in (4) and (5), we have evaluated $<H>_{min}$ as a function of the variational parameters. The kinetic and potential energy are evaluated in numerical integration using computer orientation program (MathCAD software).

The binding energy of the ground state and excited state in exciton is defined as [8]

$$E_B = E_e + E_h - <H>_{min} \quad (7)$$

Where E_B is the binding energy, E_e and E_h are the energy of electron and hole in meV, $<H>_{min}$ is minimized value of <H>.

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2.2 Photo-Ionization Cross-Section of Exciton

The excitation energy (or) photon energy dependence of the photo-ionization cross-section associated with an impurity, starting from Fermi's golden rule in the well-know dipole approximation, as in the bulk case is

$$\sigma(\hbar\omega) = \left[\left(\frac{E_{eff}}{E}\right)^2 \frac{n}{k}\right]\frac{4\pi^2\alpha}{3}\hbar\omega \times \sum_f \left|\langle\psi_f|\vec{r}|\psi_i\rangle\right|^2 \delta(E_f - E_i - \hbar\omega) \quad (8)$$

where n is the refractive index of the semiconductor, k the dielectric constant of the medium, $\alpha = \frac{e^2}{\hbar c}$ the fine structure constant, and $\hbar\omega$ photon energy, $\frac{E_{eff}}{E}$ is the ratio of the effective electric field E_{eff} of the incoming photon and the average field E in the medium. $\left|\langle\psi_f|\vec{r}|\psi_i\rangle\right|^2$ is the usually squared dipole position matrix element of an optical transition between the initial and final states $|\psi_i\rangle$ and $|\psi_f\rangle$, respectively. E_f and E_i denote, respectively, the final state energy and the initial energy of the impurity level.

$\left|\langle\psi_f|\vec{r}|\psi_i\rangle\right|^2$ is the dipole matrix element between states involved in the transition , $\vec{r}$ being the light wave polarization vector. In order to calculate the numerical values of photoionization cross-section in equation (39) the

ratio $\frac{E_{eff}}{E}$ is taken as approximately unity and the energy conserving delta function is replaced by a narrow Lorentzian

$$\delta(E_f - E_i - \hbar\omega) \rightarrow \frac{\Gamma}{\pi\left[(E_f - E_i - \hbar\omega)^2 + \Gamma^2\right]} \quad (9)$$

Where Γ is the hydrogenic impurity line-width, taken as 0.1 meV in this work [11-17] .

3. RESULT AND DISCUSSION

Some physical parameters GaAs are used here, $m_e = 0.0665m_o$, $m_{hh}^* = 0.34m_o$, $m_{lh}^* = 0.94m_o$, $\varepsilon_o = 13.2$. Where m_o is the free electron mass $(m_o = 9.1095 \times 10^{-28})$[8]. The difference of total bandgap between GaAs/$Ga_{1-x}Al_xAs$ is determined by the equation [4]

$$\Delta E_g = 1.155x + 0.37x^2 eV$$

Barrier height in electron $V_e = 0.65\Delta E_g \times 10^3$

Barrier height in hole $V_h = 0.35\Delta E_g \times 10^3$

The conduction band and valance band discontinuity is taken to be 65% and 35% of this bandgap difference respectively.

Figure 1 shows the variation of binding energy of heavy and light hole exciton in parabolic quantum well in ground state formed by GaAs/$Ga_{0.7}Al_{0.3}$ As as a function of well width (L), for a barrier heights corresponding to the Al composition x=0.3. The barrier heights of conduction band and valence band are calculated as 246.87 and 132.93 meV respectively. When L is increases, the binding energy also increases for both heavy and light hole exciton due to the compression of exciton wave function in the quantum well. If the L is increases further, binding energy reach a maximum value and then start to decrease rapidly due to spread out of the wave-function into the barrier of the well. It is also noted that the binding energy of heavy hole exciton is more bound compare the light hole exciton due to $m_{hh}^* > m_{lh}^*$. The peak value of binding for heavy hole exciton is observed at L = 43nm. Similarly the peak value of binding energy for light hole exciton is observed at L = 42nm. This behavior is the similar to the cases of a hydrogenic donor in potential wells of varied profiles [3, 4, 5, 7, 18, 20].

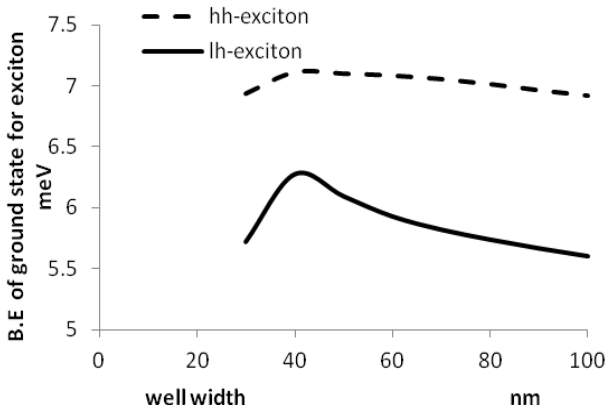

Figure - 1: Variation of the binding energy of heavy and light hole exciton for parabolic quantum well in ground state as the function of wellwidth L.

Figure 2 shows the variation of binding energy of heavy and light hole exciton in parabolic quantum well in ground state formed by GaAs/$Ga_{0.7}Al_{0.3}$ As as a function of well width (L), for a barrier heights corresponding to the Al composition x=0.3. The barrier heights of conduction band and valence band are calculated as 246.87 and 132.93 meV respectively. When L is increases, the binding energy decreases for both heavy and light hole exciton. If the L is increases further, binding energy is decrease rapidly due to spread out of the wave-function into the barrier of the well. In this case, binding energy of lh-exciton is more bounded compare that of hh-exciton for L greater than a certain critical value L_c at which they become equal. This behavior is the similar to the cases of a hydrogenic donor in potential wells of varied profiles [5, 19 and 20].

Figure 3 and figure 4 shows the variation of binding energy in ground state for heavy hole and light hole exciton in parabolic quantum well composed of GaAs/$Ga_{1-x}Al_xAs$ as the function of various Al concentrations (x=0.1,0.2,0.3,0.4,0.5) with L = 30nm,40nm. It is observed that the increase in Al concentrations, the binding energy also increases due to the barrier height increases as Al concentrations increases [21].

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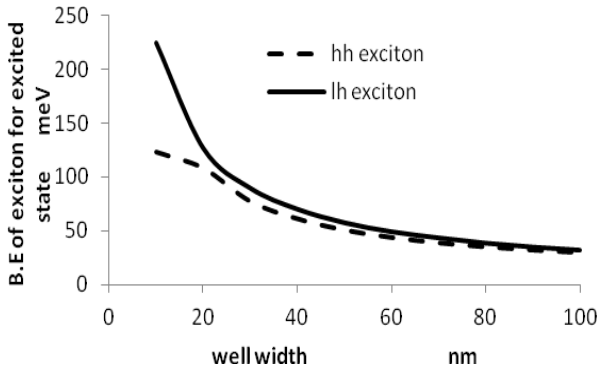

Figure- 2: Variation of the binding energy of heavy and light hole exciton for parabolic quantum well in exited state as the function of wellwidth L.

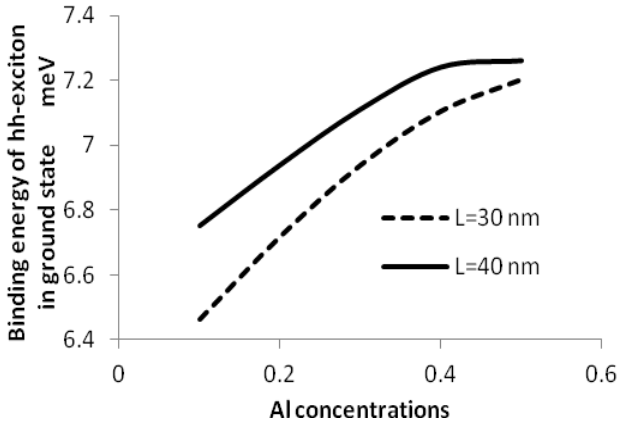

Figure -3: Variation of the binding energy in ground state for heavy hole exciton in parabolic quantum well as the function various Al concentrations(x=0.1, 0.2, 0.3, 0.4, 0.5).

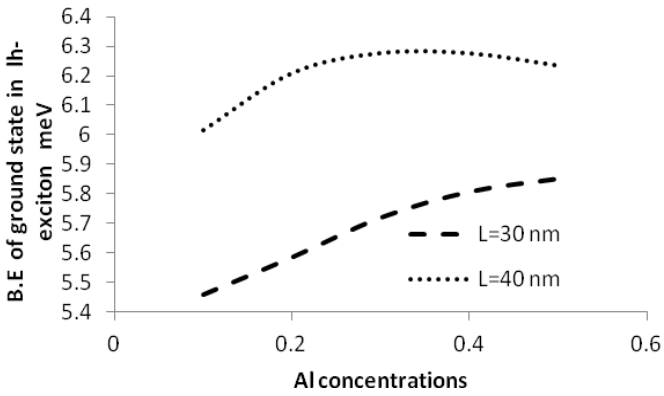

Figure -4: Variation of the binding energy in ground state for light hole exciton in parabolic quantum well as the function various Al concentrations(x=0.1,0.2,0.3,0.4,0.5).

Figure 5 shows the comparison of binding energy in heavy hole and light hole exciton in ground state with L=30nm as the function of various Al concentrations. In this case, binding energy of hh-exciton is more bounded compare that of lh-exciton due to $m^*_{hh} > m^*_{lh}$ [21].

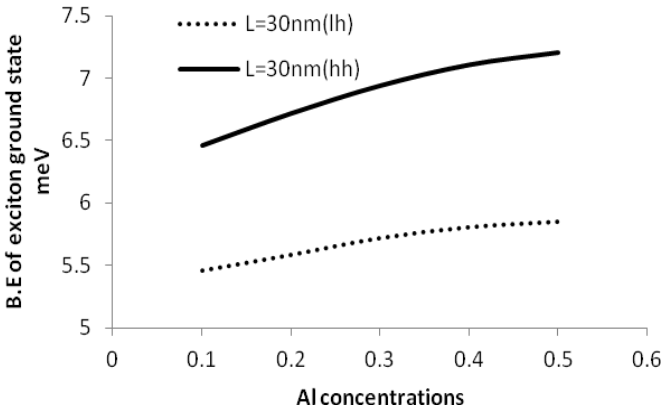

Figure- 5: shows the comparison of binding energy in heavy hole and light hole exciton in ground state with L=30nm as the function of various Al concentrations.

Figure 6 and figure 7 shows the variation of binding energy in excited state for heavy hole and light hole exciton in parabolic quantum well composed of GaAs/$Ga_{1-x}Al_xAs$ as the function of various Al concentrations (x=0.1,0.2,0.3,0.4,0.5) with L = 30nm, 40nm. It is observed that the increase in Al concentrations, the binding energy also increases due to the barrier height increases as Al concentrations increases [21].

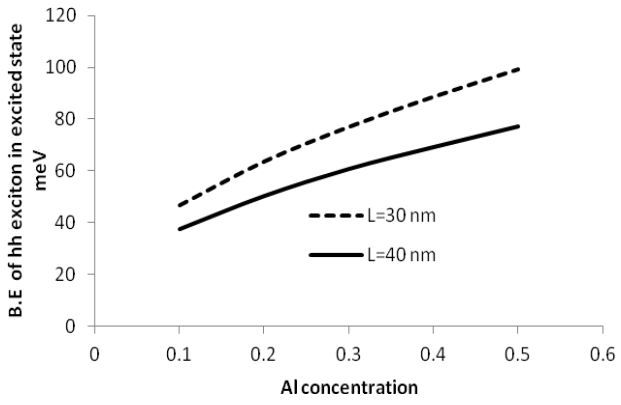

Figure -6: Variation of the binding energy in excited state for heavy hole exciton in parabolic quantum well as the function of various Al concentrations

Figure 8 shows the comparison of binding energy in heavy hole and light hole exciton in excited state with L=30nm as the function of various Al concentrations. The binding energy of lh-exciton is more bounded than that of hh-exciton due to L greater than a certain critical value L_c at which they become equal [20].

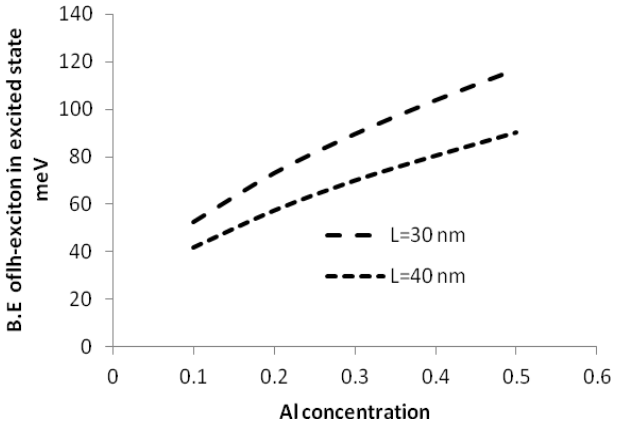

Figure -7: Variation of the binding energy in excited state for light hole exciton in parabolic quantum well as the function of various Al concentrations

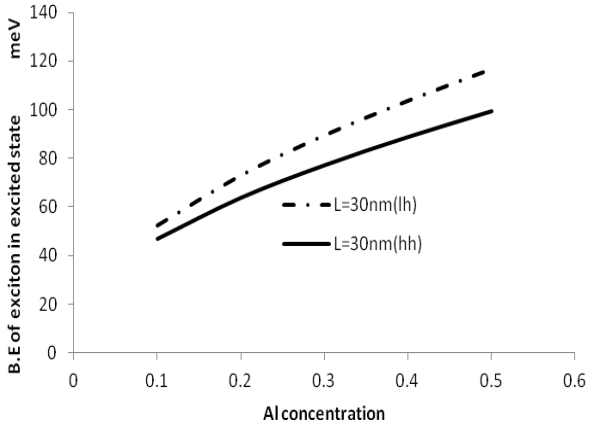

Figure -8: shows the comparison of binding energy in heavy hole and light hole exciton in excited state with L=30nm as the function of various Al concentrations.

Figure 9 shows the variation of photo-ionization cross-section in heavy hole and light hole exciton in parabolic quantum well composed of GaAs/$Ga_{1-x}Al_xAs$ as a function of the normalized photon energy $\frac{\hbar\omega}{R^*}$ (R^* is the Rydberg constant), for a barrier heights corresponding to the Al composition x=0.3. One of the most important approximations made in this work is to take the second sub-band states as the final state in the photo-ionization process. Photo-ionization cross-section of exction decreases with increases of photon energy due to ions ejection in the surface of the quantum well. Photon energy dependence of the photo-ionization cross-section is mainly due to the sizes of quantum well and the charge carries position, the value of the photon energy at which the cross-section reaches a maximum is equal to the photo-ionization threshold energy for any direction of the incident light polarization. In this case photo-ionization cross-section of exciton in light hole values is larger than that of heavy hole exciton due to the bound state of heavy hole and light hole exciton.

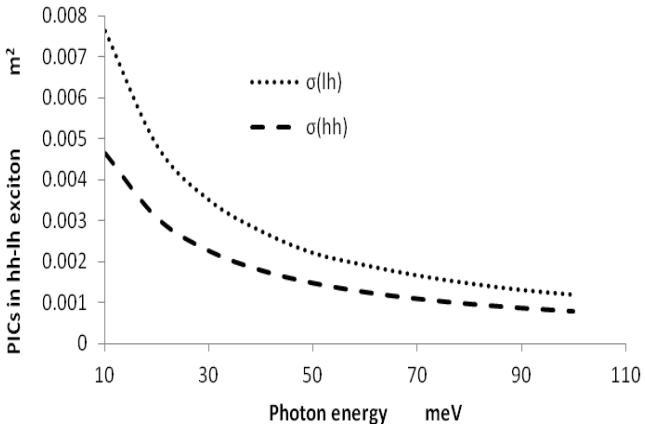

Figure -9: shows the variation of PICs for hh,lh-exciton in parabolic quantum well as the function of photon energy.

Figure 10 and 11 shows the variation of photo-ionization cross-section in heavy hole and light hole exciton in parabolic quantum well composed of GaAs/$Ga_{1-x}Al_xAs$ as a function of the normalized photon energy $\frac{\hbar\omega}{R^*}$ (R^* is the Rydberg constant), for various Al concentrations. Photo-ionization cross-section of exction decreases with increases of photon energy due to ions ejection in the surface of the quantum well. In this case barrier height is increases photo-ionization cross-section of exciton has been decreases.

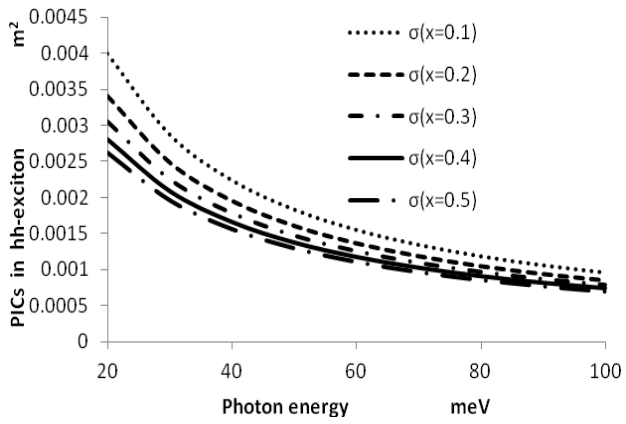

Figure -10: shows the variation of PICs for hh-exciton in various Al concentrations of parabolic quantum well as the function of photon energy.

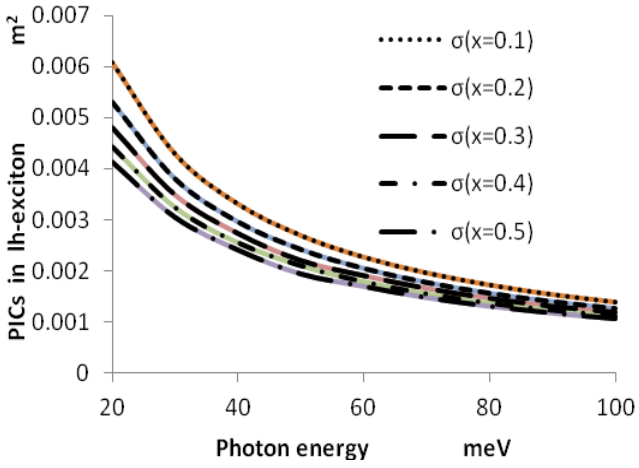

Figure -11: shows the variation of PICs for lh-exciton in various Al concentrations of parabolic quantum well as the function of photon energy.

Figure 12 and 13 shows the variation of photo-ionization cross-section in heavy hole and light hole exciton in parabolic quantum well composed of GaAs/$Ga_{1-x}Al_xAs$ as a function of wellwidth in various photon energy, for a barrier heights corresponding to the Al composition x=0.1. The barrier heights of conduction band and valence band are calculated as 77.48 and 41.72 meV respectively. Photo-ionization cross-section of exction increases with increases wellwidth reason width of quantum well increases the cross-section also increases. In this case photo-ionization cross-section of exction decreases with increases photon energy due to ions ejection in the surface of the quantum well.

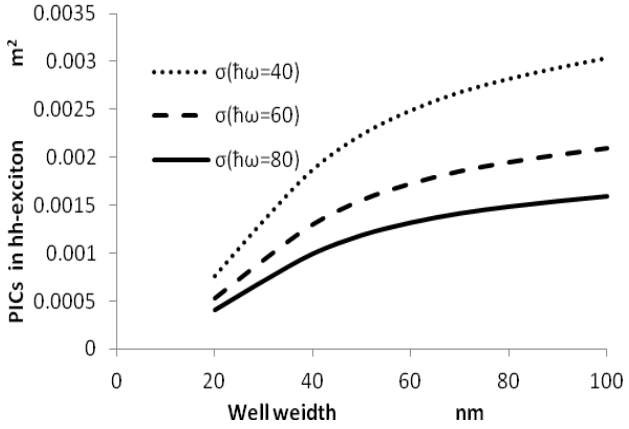

Figure-12: shows the variation of PICs for hh-exciton in various photon energies of parabolic quantum well as the function of wellwidth.

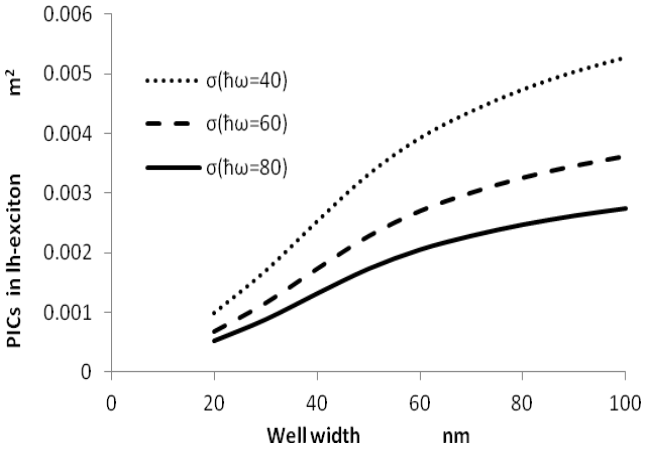

Figure-13: shows the variation of PICs for lh-exciton in various photon energies of parabolic quantum well as the function of wellwidth.

4. CONCLUSIONS

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