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Effect of Applied Electric Field on Electronic Transitions in ZnO Quantum Well

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Abstract: In this paper, we numerically investigate the impact of an electric field variation on the inter subband transitions in ZnO/MgZnO quantum well within the effective mass approximation. By solving the coupled equations Schrodinger and Poisson, we compute the energy levels, the confining potential and the wave functions. In addition we have calculated the optical absorption $\alpha_{23}(\omega)$ between the second and third excited levels E_2 and E_3. Our theoretical findings show that the ΔE_{23} transition can be adjusted by varying the electric field intensity. The obtained results are very useful to the design and growth of semiconductors materials used in resonant tunneling diodes.
Keywords: self-consistent calculation, ZnO/MgZnO quantum well, optical absorption coefficient

INTRODUCTION

In recent years, a great attention has been concentrated on the electronic transition and optical absorption coefficients in ZnO and GaNquantum wells based on wurtzite semiconductors due to their importance and various applications in electronics domain such as resonant tunneling and laser diodes, photodetectors and switches [1-4]. The optical absorption due to the electronic transitions in n-doped semiconductors quantum wells, wires and dots showed a major importance due to the higher values of the dipole matrix elements. The dipole elements are responsible on the resonance condition between different energy levels.

In the recent years, ZnO based semiconductors materials like MgZnO/ZnO and CdZnO/MgZnO have been the focus of theoretical and experimental research. They are proposed as best alternate wide band-gap semiconductors because they present several advantages compared to GaN related materials. In addition, recent experimental findings show that it's possible to observe quantum hall effect in ZnMgO/ZnO with large mobility [5, 6]. In this paper, we investigated the effect of an external electric field on the electronic transitions and optical absorption coefficient between the energy levels E_2 and E_3. Our numerical results show that the optical absorption can be altered by adjusting the intensity of the external electric field. Especially, the transition between E_2 and E_3 becomes possible for a specific value of the external electric field. Our paper is organized as follows: in section 2, we present our theory and we outline the numerical method of resolution. In section 3, we discuss the obtained results. The conclusions are given in section 4.

THEORY

We consider in this work a single quantum well $Mg_xZn_{(1-x)}O/ZnO$ under an external electric field. Using the effective mass approximation, the motion of an electron moving in z direction is given by the following equation [7-10]:

$$-\frac{\hbar^2}{2m^*}\frac{d^2\Psi_i(z)}{dz^2}+(E_C(x)+V_H(z)+V_{xc}(z)+e(F_{\text{int}}+F_{ext})z)\Psi_i(z)=E_i\Psi_i(z) \qquad (1)$$

In the equation 1, $E_C(x)$ represents the conduction band offset between ZnO quantum well and MgZnObarrier which depends on magnesium composition x and can be calculated with the following analytical expression [10]:

$$E_C(x)=0.75\,[E_g(Mg_xZn_{(1-x)}O)-E_g(ZnO)] \quad (eV) \qquad (2)$$

F_{ext} is the external electric field applied along the structure and F_{int} denotes the internal electric field produced by the piezoelectric charges accumulated at each interfaces and is given as follows [11]:

$$F_{\text{int}} = \begin{cases} \dfrac{2L_b P_{tot}}{2L_b\varepsilon_w + L_w\varepsilon_b} & in\ the\ quantum\ well \\ -\dfrac{L_w P_{tot}}{2L_b\varepsilon_w + L_w\varepsilon_b} & \text{in } the\ barrier \end{cases} \quad (3)$$

ε_b and ε_w denote the dielectric constants in MgZnO barrier and ZnO quantum well, respectively. P_{tot} Represents the total polarization (piezoelectric and spontaneous polarizations): $P_{tot} = -0.034x + 0.066x = 0.032x$ [11]. The second term in equation 1 is the Hartree potential $V_H(z)$ which describes electrostatic interaction between electrons and ions. It can be computed by solving Poisson equation using the finite difference method:

$$\frac{d^2V_H(z)}{dz^2} = \frac{4\pi e^2}{\varepsilon}[N_D(z) - n(z)] \quad (4)$$

In the Poisson equation, $n(z)$ represents the density of the free electrons in the whole structure. The barriers are uniformly doped with donor impurities having the concentration $N_D(z)$. The electronic density of free electrons can be written as follows:

$$n(z) = \sum_i \frac{m^* K_B T}{\pi\hbar^2} L\log[1+\exp(\frac{E_F - E_i}{K_B T})]\Psi_i^2(z) \quad (5)$$

In the previous equation, K_B is the Boltzmann constant, E_F denotes the Fermi level and m^* is the effective mass of the electron and T is the absolute temperature. All the previous equations are coupled. So, they are numerically solved using the finite difference technique [10]. After the subband energies and their corresponding wave functions are obtained, the linear and third-order nonlinear optical absorption coefficient describing an inter subband transitions between the initial and final states $(E_i \to E_f)$ can be clearly calculated as follows [10]:

$$\alpha^1(\omega) = \omega\sqrt{\frac{\mu}{\varepsilon}} \times \frac{|M_{21}|^2 \sigma_v \hbar/\tau_{in}}{(\Delta E - \hbar\omega)^2 + (\hbar/\tau_{in})^2} \quad (6)$$

$$\alpha^3(\omega) = -2\omega\sqrt{\frac{\mu}{\varepsilon}}\left(\frac{I}{\varepsilon_0 n_r c}\right) \times \frac{|M_{21}|^4 \sigma_v (\hbar/\tau_{in})}{[(\Delta E - \hbar\omega)^2 + (\hbar/\tau_{in})^2]^2} \times \left(1 - \frac{|M_{22} - M_{11}|^2}{|2M_{21}|^2} \cdot \frac{(\Delta E - \hbar\omega)^2 - (\hbar/\tau_{in})^2 + 2\Delta E(\Delta E - \hbar\omega)}{(\Delta E)^2 + (\hbar/\tau_{in})^2}\right) \quad (7)$$

Here, $M_{fi} = \int_{-\infty}^{+\infty} \psi_f^*(z)\, z\, \psi_i(z) dz$ represents the matrix element. $\Delta E = E_f - E_i$. The Fermi occupancy function is given by: $\sigma_v = \ln\left\{\dfrac{1+\exp[(E_F - E_0)/K_B T]}{1+\exp[(E_F - E_1)/K_B T]}\right\}$. μ denotes the permeability, c is the speed of light, $\tau_{in} = 0.24\,ps$ represents the intrasubband relaxation time, and I is the intensity of light . Using Equations (7) and (8), we calculate the total absorption coefficient as $\alpha(\omega) = \alpha^1(\omega) + \alpha^3(\omega)$. The physical parameters used in our simulations are [12]: $m^* = (0.23 + 0.05x)m_0$, $\varepsilon(x) = 8.1 + 1.5x$, $I = 1.0\,MW/cm^2$, $\mu = 4\pi \times 10^{-7}\,H.m^{-1}$ and $T = 300\,K$. The quantum well and barrier have the same widths $L_w = L_b = 6.5\,nm$. The concentration of impurities is fixed to $N_D = 5 \times 10^{19}\,cm^{-3}$

RESULTS AND DISCUSSION

Figures 1, 2 show the effects of magnesium composition x on the ground, first and the second wave functions and the confining potential in MgZnO/ZnO single quantum well. As expected, when we change the magnesium composition, the energy levels are modified. Especially, they increase because the confining potential becomes deeper. In

addition, we remark that all the wave functions present an asymmetric profile. This asymmetry of the wave functions leads to a localization of the electrons near the left side of the quantum well. On the other hand, we remark that the bottom of ZnO quantum well is more tilted when we increase the magnesium composition. This inclination observed in the profile of the confining potential along the structure is due to the strong intensity of the internal electric field which is produced by piezoelectric charges accumulated at each interface between ZnO quantum well and barriers. Note that the piezoelectricity in these materials is an important phenomenon and has a great effect on the optical absorption. On the other hand the internal electric field can produces a 2DEG gas at the left interface between the quantum well and the barrier that can be used for various applications in optoelectronics domain such as the high speed devices.

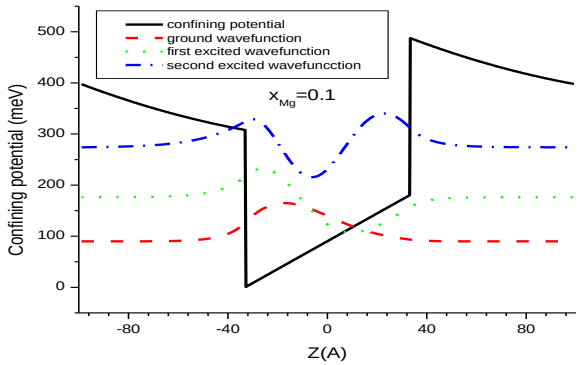

Fig-1: Confining potential as a function as the growth axis z for x =0.1

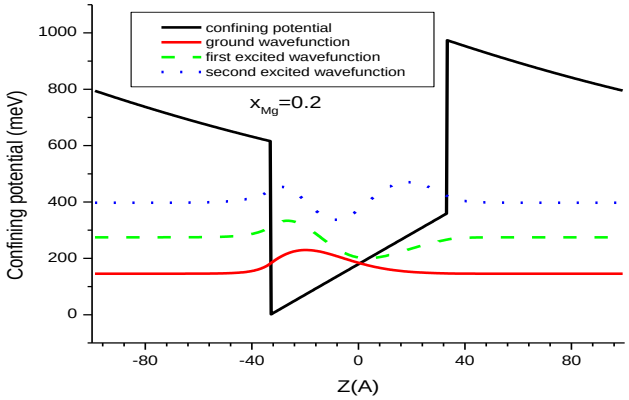

Fig-2: confining potential as a function as the growth axis for x=0.2

In figures 3, 4, 5, we present the optical absorption coefficients as a function of the incident photon energy for three values of electric field $F = 500\,KV/cm, 800\,KV/cm$ and $1200\,KV/cm$. From these figures, we remark that when we increment the values of F, the maximum of all optical absorption coefficients move toward lower energies (red-shift). We remark that the amplitudes $\alpha_{12}(\omega)$ and $\alpha_{13}(\omega)$ decrease by increasing F. However $\alpha_{23}(\omega)$ which is forbidden for $F = 0\,KV/cm$, becomes possible by increasing progressively F and reaches the value $2000\,cm^{-1}$ for $1200\,KV/cm$. The effect of the electric field on the wave functions Ψ_1, Ψ_2 and Ψ_3 is presented in figures 6, 7 and 8. We remark from these figures that by increasing the intensity of electric field, the wave functions become more symmetric in the ZnO quantum well. The symmetry of the wave functions is due to the symmetry of the confining potential. In fact, when the electric field is equal to $500\,KV/cm$ the potential presents an inclination with higher slope along the quantum well. Thus, the wave functions are localized near the left side of the quantum well. However, by increasing the magnitude of the electric field, the slope of the inclination of the confining potential will be reduced, and for $F = 1200\,KV/cm$ the confining potential becomes almost flat in the quantum well region, consequently the wave

functions are spread entire the ZnO layer. In addition, we remark that the energy positions are decreased when we increment F which confirms the red shift behavior of the optical absorption coefficient.

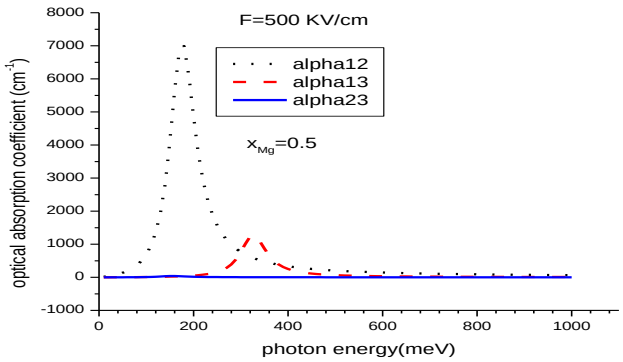

Fig-3: Optical absorption coefficients as a function of incident energy (F=500Kv/cm)

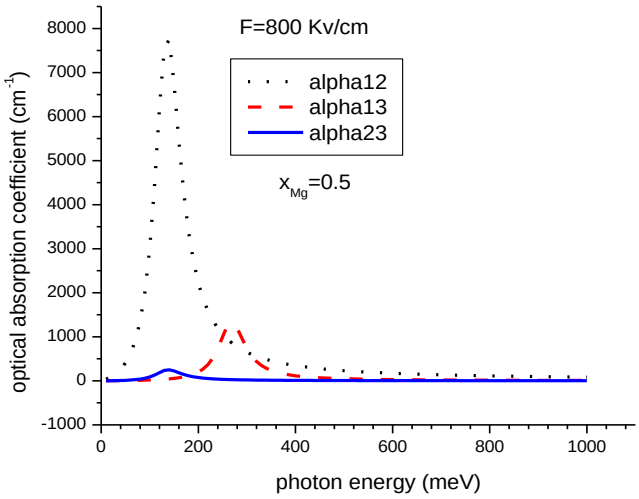

Fig-4: Optical absorption coefficient as a function of incident energy (F=800 Kv/cm)

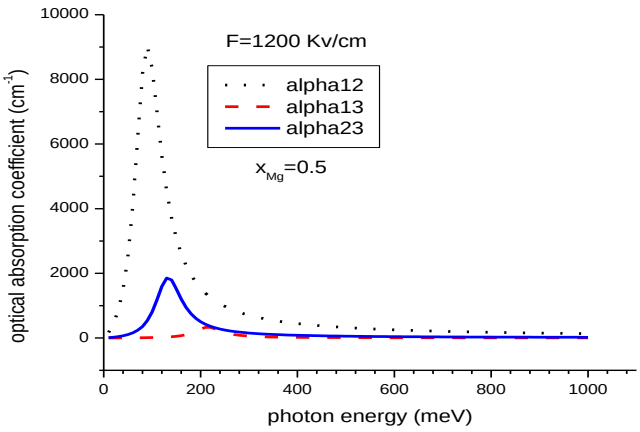

Fig-5: Optical absorption coefficients as a function of incident energy (F=1200Kv/cm)

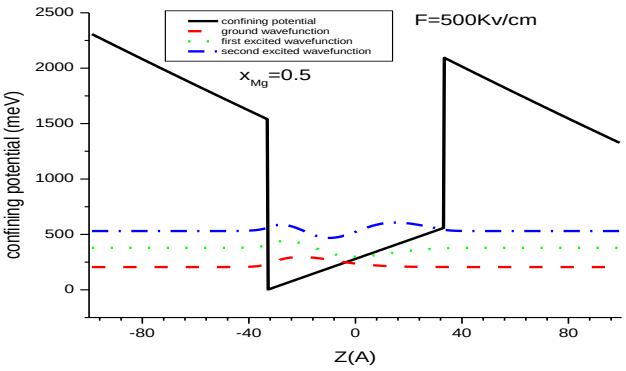

Fig-6: Confining potential and wavefunctions for applied electric field F=500Kv/cm

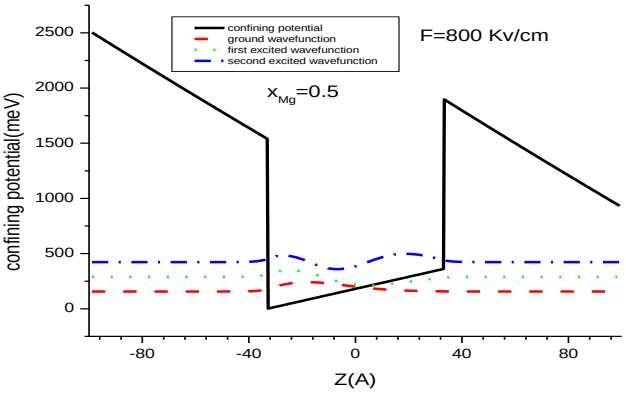

Fig-7: Confining potential and wavefunctions for applied electric field F=800Kv/cm

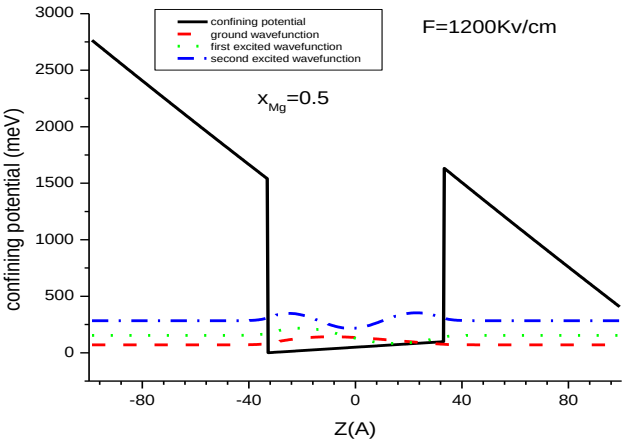

Fig-8: Confining potential and wave functions for applied electric field F=1200Kv/cm

CONCLUSION

In this paper, the effects of external electric field on the optical absorption coefficients are investigated for an MgZnO/ZnO single quantum well using the effective mass approximation. The applied electric field modifies the confining potential, the electronic wave functions and accordingly the energy positions. When these electronic properties are affected, all the optical absorptions coefficients are changed. We obtain the blue and the red shift by varying the magnesium composition and the magnitude of the electric field. In addition, we found that some inter subband transitions

are very sensitive to the external electric field. This later can overcome the internal field produced by the piezoelectric charges accumulated at each interface between ZnO quantum well and MgZnO barrier. Finally we have demonstrated that the forbidden optical absorption coefficient $\alpha_{23}(\omega)$ becomes possible by increasing the magnitude of the electric field. The obtained results enhance the possibility of the design and fabrication of various devices used as optical filters tuned by an applied electric field.

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