Effect of conduction band non-parabolicity on the intersubband transitions in ZnO/Mg,Zn1-xO quantum well heterostructures

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Abstract. In this paper, we have calculated the electronic states and the coefficient of transmission in ZnO/Mg,Zn1-xO quantum well structures (QW), with 20% of Magnesium in both the parabolic and the non-parabolic cases. Our calculations are performed in the context of the approximation of the envelope function formalism, and using the finite difference method. The results show that the intersubband transition energy increases rapidly with well width until \( L_w=5\)nm and becomes almost constant (specially transitions \( E_{13} \) et \( E_{23} \)). Wavelength \( \lambda_{23} \) decreases with well width until \( L_w=5\)nm and becomes constant. The non-parabolicity effect is more pronounced for small QW \( (L_w \leq 5\)nm\) and less marked in narrow and large QW. Also, we are studied the coefficient of transmission. We notice that when the height of barrier increases the coefficient of transmission decreases. It will be necessary to provide more energy to the electron so that it can cross the barrier. We also notice the variations related to a phenomenon of reflection quantum.

1. Introduction:
Semiconductor materials II-VI with a large band gap of the ZnO/MgZnO system are gaining increasing interest; they are the potential competitors of the other large family of materials with a large band gap, the III-V nitrides. Like the nitrides, ZnO crystallizes in the wurtzite phase then the presence of the particular effects related to the polarization with internal electric fields more intense than those in the nitrides III-V, due to their applications in the field of fabrication of the photodetectors and diode lasers [1-5]. However, ZnO has several advantages, the ZnO substrate is naturally solid ZnO of good crystalline quality, it is not very expensive and easy to manufacture [6-7]. Intersubband transitions in quantum wells of ZnO/MgZnO are theoretically and experimentally determined for the purpose of improving optoelectronic properties, and making it an ideal candidate for optoelectronic devices, more precisely in the ultraviolet regions [8-11].

Recently, several groups interested on intersubband transitions in quantum wells composed of semiconductors due to their potential in ultraviolet regions. We found that Bhattacharya et al.[12] experimentally studied the transmission spectra of MgZnO thin films with different Mg to Zn by changing the thicknesses of ZnO layer, and found that the films showed high (>80%) transparency, and the absorption edge shifted as the thickness of the ZnO sublayers decreases. Ohno et al.[13-14] studied the intersubband transitions in ZnO-MgZnO and have reported that there are unique properties for intersubband absorption in ZnO quantum well. In this work, we adopt a numerical method to determine the intersubband transitions of the conduction band in ZnO/MgZnO, by solving the Schrödinger equation, under the effect of the approximation of the envelope function and considering the impact of
the polarization electric fields in the quantum wells and barriers. In Part 2, we present the study of the calculations of the structure of the band and show the effects of non-parabolicity on the positions of confined levels. In Part 3, we present the study of the transmission coefficient.

2. General formalism:

Under the effect of the approximation of the envelope function, the wave functions and the energy levels are obtained by solving the Schrödinger equation:

$$\left( \frac{p^2}{2m_0} + V(r) + U_H(z) \right) \psi(r) = E \psi(r)$$  \hspace{1cm} (1)

Where $V(r)$ is the crystalline potential and $U_H(z)$ is the potential of the heterostructure.

$$U_H(z) = \begin{cases} eF_b z - eF_w (z_2 - z_1) + \Delta E_c & z < z_1 \\ eF_w (z - z_1) & z_1 \leq z \leq z_2 \\ eF_b (z - z_3) + \Delta E_c & z > z_2 \end{cases}$$  \hspace{1cm} (2)

Where $z_1$ and $z_2$ determine the barrier and well interfaces positions: $z_1 = z_2 + z_1$. The position $z_1$ taken as the origin of the potentials.

The potential of a heterostructure $U_H(z)$ often results from the strip discontinuity ($\Delta E_c$: offset) at the interface of the two materials due to the difference in the position of the conduction bands. Nevertheless, this time, the presence of internal electric fields ($F_w$ and $F_b$) in each of the two materials will influence it.

$$F_w = \frac{(P_b - P_w) L_b}{\varepsilon_0 (\varepsilon_w L_w + \varepsilon_b L_b)} \quad \text{and} \quad F_b = \frac{- (P_b - P_w) L_w}{\varepsilon_0 (\varepsilon_w L_w + \varepsilon_b L_b)} = - F_w \frac{L_w}{L_b}$$  \hspace{1cm} (3)

Where $\varepsilon_0$, $\varepsilon_w(b)$ and $P_w$ $P_b$ are respectively the free static dielectric constant, the static dielectric constant of the well (barrier) and the total polarizations in the well and in the barrier [15-16].

The maximum value of the internal electric field $F_{\text{MAX}} = \frac{\Delta P}{\varepsilon_b}$ therefore depends directly on the magnesium proportion in the barrier. An approximately linear increase was measured by time-resolved photoluminescence measurements [17].

$$F_{\text{MAX}} \left( x_{Mg} \right) = 3.95 x_{Mg} \text{ MV/cm} \quad \text{That to say} \quad F_{\text{MAX}} = 0.79 \text{ MV/cm}$$

The effective mass, the relative permittivity are calculated from Vegard’s law (linear interpolation between the values of ZnO and MgO) and the gap varies with the composition according to the quadratic law:
Where the bowing parameter \( b = 0 \) eV for the MgZnO alloy where the Mg fraction is less than 36\% [18]. Moreover \( \Delta E_c = 0.7 \Delta E_g = 210 \) meV.

The numerical resolution is based on the finite difference method. It considers the structure as a succession of \( n + 1 \) layers of very small but equal thicknesses, \( \Delta z \). In each layer, the mass (\( m_n \)), the potential (\( U_n \)) and the envelope functions (\( \chi_n \)) are considered as constants. The envelope functions in the different layers in this model are linked together by:

\[
\chi_{n+1}(z) = \frac{1}{\sqrt{m_{n+1}}} \left[ \int_{z}^{Z_n} \frac{1}{\sqrt{m(z)}} \frac{d}{dz} \left( \frac{d}{dz} \chi(z) \right) \right] \chi_n(z)
\]

The Schrödinger equation is reduced to the following differential equation:

\[
\left( -\frac{\hbar^2}{2} \frac{d^2}{dz^2} \left( \frac{1}{m(z)} \frac{d}{dz} \right) + U(z) \right) \chi(z) = E \chi(z)
\]

The calculations were developed in the parabolic approximation and in the nonparabolic case where the effective mass depends on the energy according to the Nilson model [19]:

\[
m_{w,b}(\varepsilon) = m_0 \left( 1 \pm \frac{\varepsilon}{E_{w,b}} \right) \quad \text{and} \quad m_{w,b}(\varepsilon) = m_0 \left( 1 - \frac{V_b - \varepsilon}{E_{w,b}} \right)
\]

Table 1: Structural and electronic parameters of ZnO and MgO [19].

| Parameter               | ZnO     | MgO     |
|-------------------------|---------|---------|
| Lattice constant \( a \) (Å) | 3.2     | 4.2     |
| Gap energy (eV)         | 3.37    | 5.4     |
| Conduction band effective masses \( m_e \) | 0.28    | --      |

\( E_{w,b} \): The gap energy of the well (barrier)
\( m_{w,b} \): The effective mass of BC electrons in the parabolic approximation in the well (barrier)
\[ X_{n+1} = X_n \left( \Delta k + \frac{m_n}{m_{n+1}} \right) \frac{m_n}{m_{n+1}} X_{n-1} \]  \quad (7)

Where:
\[ k_n = \frac{2 m_n (U_n - E)}{\hbar^2} \]

3. Result and Discussion:

3.1 Electronic states in ZnO/MgxZn1-xO quantum well

The confined levels are relatively sensitive to variation in the width of the barrier, in particular for low \( L_b \). The positions of the fundamental level and the 1\(^{st}\) excited level, located below \( V_s \), increase when the barrier is widened. On the contrary, those located in above of \( V_s \) descend in energy. It should be noted that those energies variations are generally low after a certain width of the barrier. Considering, as well, the value of \( L_b = 8 \) nm to study the effect of the well width. The following figure is a graphical representation of the different confined levels evolution and transitions energies in function of well width \( L_w \):

![Graphical representation of the different confined levels evolution and transitions energies in function of well width \( L_w \).](image)

According to the curve in figure 2. (a), it can be seen that when the well width decreases each confined levels increase in energy up to a certain width, which they have a maximum value and below which their energies decrease, \( L_w = 45 \) Å for \( E_3 \) And \( L_w = 25 \) Å for \( E_2 \). When a confined level energy enters in above of \( V_s \) its position undergoes a slowdown due to the combined effect of the continuum and confining field of the barrier. In addition, for broad well widths of the variation of confined levels energies are overall weak.
Figure 2. (a): Evolution confined levels depending the width of the well to $L_b = 8$nm. (b): The transitions energies depending of the well width to $L_b = 8$nm.

For the nonparabolicity, its effect is negligible for the fundamental level. The $E_{1p}$ and $E_{1n}$ are almost coinciding. But each time the level is excited the nonparabolicity effect becomes important; it lowers the confined level energy for wells immense, about $\approx 2.8$eV for $E_2$ and $\approx 8$eV for $E_3$. Thus, for fine wells the nonparabolicity effect is generally low.

From the figure 2. (b), it can be seen that each transition has two regions of variation, one where a transition increases with $L_w$, and the other where it decreases. In the 1st region, the upper level exists above $V_s$ moves slowly, unlike the level below $V_s$ decreases sharply, which resulting an increase in transition energy. In the second region, both levels have lower positions than $V_s$, the changes in transition energy has a usual behavior corresponding to a decrease, but this decreasing is lower than first. Between $L_w = 10-20$ Å, The transition $E_{23}$ as a function of the well width remains practically constant. Indeed, the two Levels are located above $V_s$, where the displacement of the levels is low, with a variation almost similar. $E_{12}$ calculations cover the range of the midinfrared wavelengths in the far infrared ($\lambda_{12} = 9—16$ μm).

Thus, those transitions have a maximum. The transition $E_{13}$ has the highest, $E_{13} = 194.5$ meV for $L_w = 50$ Å corresponds to $\lambda_{13} = 6.37$ μm. concerning the field térahzétique the transition $E_{23}$ allows us this emission/detection for the geometries with will width less than $L_w = 35$ Å, $\nu_{23}$ relaxes from 1.1 THz to 10 THz.
Figure 3. Evolution of the frequency of the transition $E_{23}$ as function as the width of the well.

The nonparabolicity reduces the transitional energies because of its effect on the confined levels positions, thus, for large wells, it drop the transition energy $E_{13}$ by about $\approx 6 \text{ eV}$ and the transition $E_{12}$ by about $\approx 3 \text{ eV}$. However, for fine wells the effect of nonparabolicité is generally low, the transition energy $E_{13}$ down by about $\approx 0.5 \text{ eV}$. Ours results are in good agreement with [19, 20, 21].

4. Transmission

4.1 Transmission in ZnO/MgZnO quantum well

We consider a ZnO / MgZnO heterostructure to study the tunnel effect through this structure as shown in the figure below.

The transmission coefficient of an electron through the potential barrier is written as [19]:

$$T(E) = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)} \frac{\hbar^2}{m} \left(\frac{L_0}{\hbar} \sqrt{2m(V_0 - E)}\right)}$$

(8)
With $E$ the electron energy, $V_0$ the barrier height, $L_b$ its width and $m$ the electron mass.

Different variables are involved in the calculation of transmission coefficient: the barrier thickness, the electron energy or the height of the barrier. We have shown in the following figures (Figure 4 and Figure 5), the influence of two parameters on the transmission coefficient: the thickness and height of the potential barrier.

**Figure 4.** The coefficient of transmission of a simple layer of MgZnO with 20% of Mg according to thickness of the layer with $V_0=0.26$ eV.

**Figure 5.** The coefficient of transmission of a simple layer of MgZnO, thickness $L_b=8$ Nm According to $X$ fraction of Mg.
Generally, in figure 4, the wider the barrier, the transmission of an electron with a given energy will be lower. When the thickness of the barrier is 5nm, very few electrons can pass through it (coefficient close to 0 when the energy is less than 0.26 eV). When the thickness is less than 5 nm, we see that the transmission coefficient is no longer zero for energies lower than the barrier height. The probability of tunneling increases. Beyond the barrier energy (0.2 eV), we observe on the thickest barrier, oscillations related to a phenomenon of quantum reflection.

Figure 5. Indicates that there is a decrease in the transmission coefficient when the barrier height increases (the fraction of Mg increases). In this case, it will be necessary to provide more energy to the electron so that it can cross the barrier. Beyond the barrier energy ($V_b$), we also notice variations related to a phenomenon of quantum reflection.

![Graph showing transmission coefficient vs energy for parabolic and non-parabolic cases](image)

**Figure 6.** The transmission coefficient in the parabolic and non-parabolic cases, $L_b = 8$nm And $V_b = 0.526$ eV.

The both samples present a good optical transmission around 90%, in most cases; thin multilayers have shown different physical properties. The variation of the shape of the individual MgZnO layers has a significant influence on the optical properties and the crystal structure of the MgZnO alloys. It can be seen that the transmission in the case of the parabolic bands are made in a fast way than in the non-parabolic bands. A good agreement is obtained with the existing literature values.
5. Conclusion
We have studied the conduction band profile and carried out calculations of the transitions energies in a quantum well ZnO/MgZnO with 20% of magnesium and for geometries 8/1-8/8 nm. Three levels of energy could be confined within a certain widths leading to three permissible transitions because the selection rules are changed (Asymmetric wells). We considered how the material parameters such as non-parabolicity affect those energies and wavelengths corresponding. The transition E_{12} cover the range of the mid-infrared wavelengths to the far infrared (λ_{12}≈9-16 μm). Our results show that the transition energies E_{12} of the quantum well structures ZnO/MgZnO, which have very close mesh parameters, in advantageous to have an unconstrained structure, gave terahertzic frequencies ν for the barrier is fine. We also have enregistered the variations related to a quantum reflection phenomenon.

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