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Determination of the Electronic Energy Levels of a Quantum well Heterostruture $Zn_{1-x}Mg_xO/ZnO/Zn_{1-x}Mg_xO$

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Authors' contributions

This work was carried out in collaboration among all authors. Authors MT and AD designed the study, performed the statistical analysis, wrote the protocol, and wrote the first draft of the manuscript. Authors BBA, BLO, OAN MD and AB managed the analyses of the study. Author BBA, BLO, OAN MD and AB managed the literature searches. All authors read and approved the final manuscript.

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ABSTRACT

This paper studies a quantum well heterostructure made up by a zinc oxide (ZnO) thin layer (well) sandwiched between two $Zn_{1-x}Mg_xO$ layers acting as potential barriers. Setting the width of the well to a = 10 nm, the allowed quantum states in the conduction band (CB) and the wave function profiles are examined for two values of magnesium concentration : x = 0.1 and x = 0.2. The calculated wavelengths corresponding to intra-band transitions in the conduction band are in the infrared domain of the electromagnetic spectrum. These wavelengths depend on x, allowing to control the optoelectronic properties of the quantum well by adjusting the concentration x during the growth process.

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1. INTRODUCTION

In the last few years, semiconductors based quantum well structures have been intensively investigated because of their interesting optical and electrical properties. From the years 70, the investigations showed that lasers whose active layer is very thin "quantum well" would be more efficient than lasers with massive active layer [1]. The first quantum wells were formed from a $GaAs$ layer interposed between two barriers made of $AlAs$ layers [2]. Nowadays, quantum wells are mainly manufactured by Molecular Beam Epitaxy "MBE" or by Chemical Vapor Deposition "CVD" [3].

The present article studies a quantum well structure made up by zinc oxide (ZnO), a semiconductor with a large fundamental band gap of about $3.37\,eV$ and an exciton banding energy of $60\,meV$ at room temperature. The material is chemically and thermally stable, non-toxic and abundant in the nature [4]. To develop a ZnO based quantum well, it is used a higher gap material like magnesium and zinc oxide ($Zn_{1-x}Mg_xO$), the most important ternary alloy of ZnO. The gap of ($Zn_{1-x}Mg_xO$) is adjustable with the concentration x and varies between $3.37\,eV$ and $6.7\,eV$ [5]. In the interval $0 \leq x \leq 0.36$, the band gap width E_g of the alloy, the effective mass m^* for the electron and the electronic affinity e_χ vary linearly with x according to Vegard's law [6,7]. The study is focused on electron behavior in a finite square quantum well $Zn_{1-x}Mg_xO/ZnO/Zn_{1-x}Mg_xO$ by analyzing the energy of the particle and the corresponding wave function. The bound states energy with the related wave function ψ will be given through solutions of transcendental equations obtained by resolving the Schrödinger equation [8,9].

2. BAND DIAGRAM OF THE HETEROSTRUCTURE

The model used for the calculations, is a simple square quantum well formed by a thin layer of ZnO sandwiched between two layers of $Zn_{1-x}Mg_xO$ which is grown along the $c\ axis$. The charges carriers of the well "electrons and holes" will be geometrically confined in the plane space formed by the ZnO layer and perpendicular to the growth direction. Taking into account the values of gap and electronic affinities of ZnO and $Zn_{1-x}Mg_xO$, the band structure of the heterostructure can be represented as shown in Fig. 1.

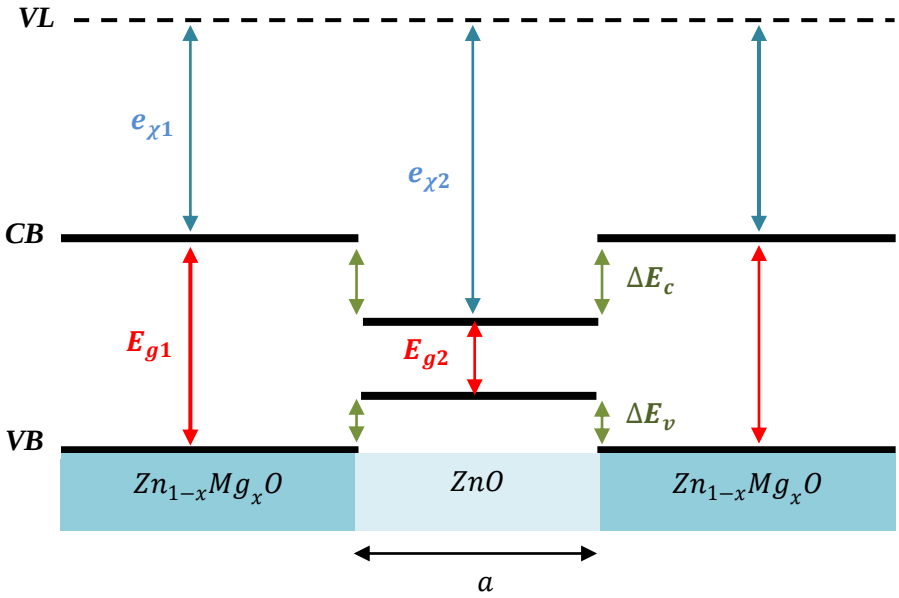

Fig. 1. Band structure of quantum well $Zn_{1-x}Mg_xO/ZnO/Zn_{1-x}Mg_xO$

Electrons and holes are confined inside the same material ZnO , so a type I quantum well is obtained. In fact, there are two distinct quantum wells whose common width corresponds to the thickness of the ZnO layer : the well of the conduction band where the electrons are confined and that of the valence band "retuned or reversed well" where the holes are locked down. This article focuses only on the well of the conduction band represented in Fig. 2.

The depth $V_0 = \Delta E_c$ of this well is given by the following relation [10] :

$$\Delta E_g = \frac{2}{3}\Delta E_c \qquad (1)$$

Electrons are considered as particles of effective mass m^* confined in a direction $z'z$ in a square potential of depth V_0 and width a bounded on $z'z$ axis by $z = -\frac{a}{2}$ and $z = +\frac{a}{2}$.

The one dimensional, time-invariant and non-relativistic Schrödinger equation governing the movement of an electron, takes the general form:

$$-\frac{\hbar^2}{2\,m^*}\frac{d^2\psi(z)}{dz^2} + V(z)\,\psi(z) = E\,\psi(z) \qquad (2)$$

The resolution of the Schrödinger equation leads to two transcendental equations which are implicit in E:

$$tan\left(k_2\frac{a}{2}\right) = \frac{k_1}{k_2} > 0 \quad \text{and} \quad cotan\left(k_2\frac{a}{2}\right) = -\frac{k_1}{k_2} < 0 \qquad (3)$$

These two equation refer to two classes of wave functions alternating from symmetrical "even" to antisymmetrical "odd" and whose union gives all the stationary states and allowed energies for $E < V_0$. Wave functions for symmetrical and antisymmetrical solutions for regions I, II and III are determined. The values of k_2 are determined graphically and give the energy by :

$$E = \frac{\hbar^2 k_2^2}{2\,m^*}$$

3. RESULTS AND DISCUSSIONS

Calculations are made for a quantum well of width $a = 10\,nm$, for two values of the composition of $Zn_{1-x}Mg_xO$: $x = 0.1$ and $x = 0.2$. The following table gives the solutions k_2 for equation (3) and the related energy levels of possible stationary states for electrons in the conduction band.

The electron confinement potential calculated from relation (1) is $V_0 = 167\,meV$, for $x = 0.1$, It is theoretically established that for a finite quantum well of depth V_0 and width a , the number of quantum states accessible to the electrons in the well is [11,12]:

$$N = 1 + Ent\left(\frac{a}{\pi\hbar}\sqrt{2m^*V_0}\right) \quad Ent \text{ the entire part} \qquad (5)$$

For $x = 0.1$, $N = 4$ states, which is in agreement with relation (5), as shown in Fig. 3.

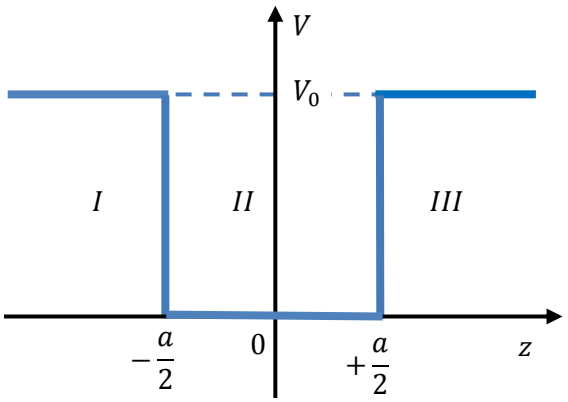

Fig. 2. Schema of a finite symmetrical square well

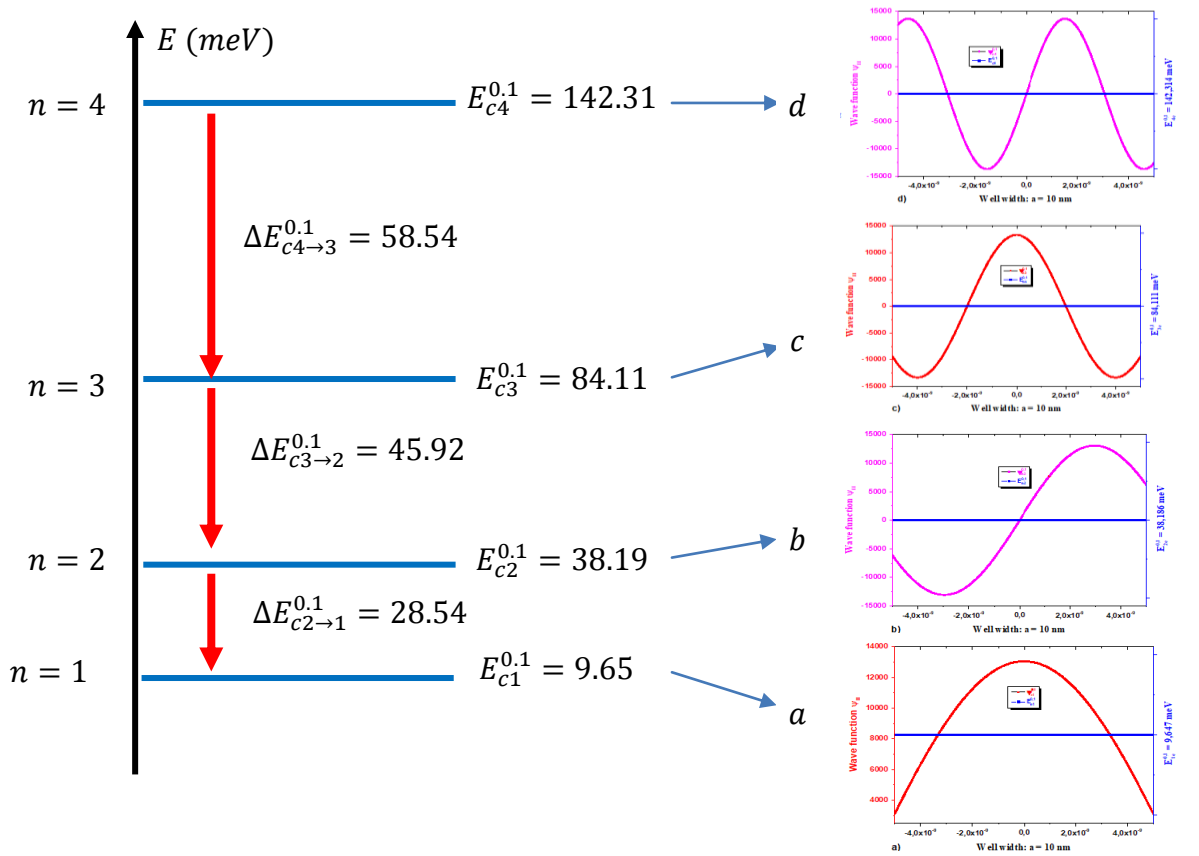

Fig. 3. Diagram for energy levels E_n and the associated wave functions profiles $\psi_{II}(z)$ in the well for $= 0.1$: (a) fundamental level ; (b) first excited state ; (c) second excited state ; (d) third excited state

The discrete energy values correspond to the energy operator H eigenvalues. This discretization of energy is justified by the nanometric dimensions confirming the quantum character of the system. The wavelengths corresponding to the inter sub-band transitions represented in Fig. 3, are: $\lambda_{c2\to1}^{0.1} = 43.49\,\mu m$; $\lambda_{c3\to1}^{0.1} = 27.03\,\mu m$; $\lambda_{c4\to3}^{0.1} = 21.32\,\mu m$. The energy levels are not equidistant : the interval between two successive ones increases with excitation, which justifies the progressive reduction of the corresponding wavelengths which lie in the far infrared range from $20\,\mu m$ to $1\,mm$ of the electromagnetic spectrum. For the direct transition between the last excited state and the ground state, the corresponding radiation from the desexcited photon energy is $\lambda_{c4\to1}^{0.1} = 14.97\,\mu m$. The wave functions of these four quantum levels are shown in Fig. 3 and illustrate the confinement of electrons in the well of the conduction band with four accessible quantum states. These four states are associated to two even wave functions (a) and (c) and to two odd wave functions (b) and (d). The even functions correspond respectively to the energy levels $E_{c1}^{0.1} = 9.64\,meV$ and $E_{c3}^{0.1} = 84.11\,meV$. They have respective amplitudes $|\psi_{c1_{max}}^{0.1}| = 13.06 \times 10^3$ and $|\psi_{c3_{max}}^{0.1}| = 13.32 \times 10^3$ reached at the center $(z = 0)$ of the well. The two odd functions (b) and (d) are associated with the energy levels $E_{c2}^{0.1} = 38.19\,meV$ and $E_{c4}^{0.1} = 142.31\,meV$ with the respective amplitudes $|\psi_{c2_{max}}^{0.1}| = 13.06 \times 10^3$ and $|\psi_{c3_{max}}^{0.1}| = 13.67 \times 10^3$. Generally, the amplitude of the wave functions increases with excitation. The curves show the presence of nodes for the excited states and the number of nodes increases with the energy level according to the formula $n \longrightarrow 1$ [13]. It is noted that wave function spreads out beyond the well, by penetrating in the classically forbidden region and therefore reduces its kinetic energy.

For $x = 0.2$, the calcul of confinement potential gives $V_0 = 335\,meV$ and the roots of transcendal equation are listed in Table 2.

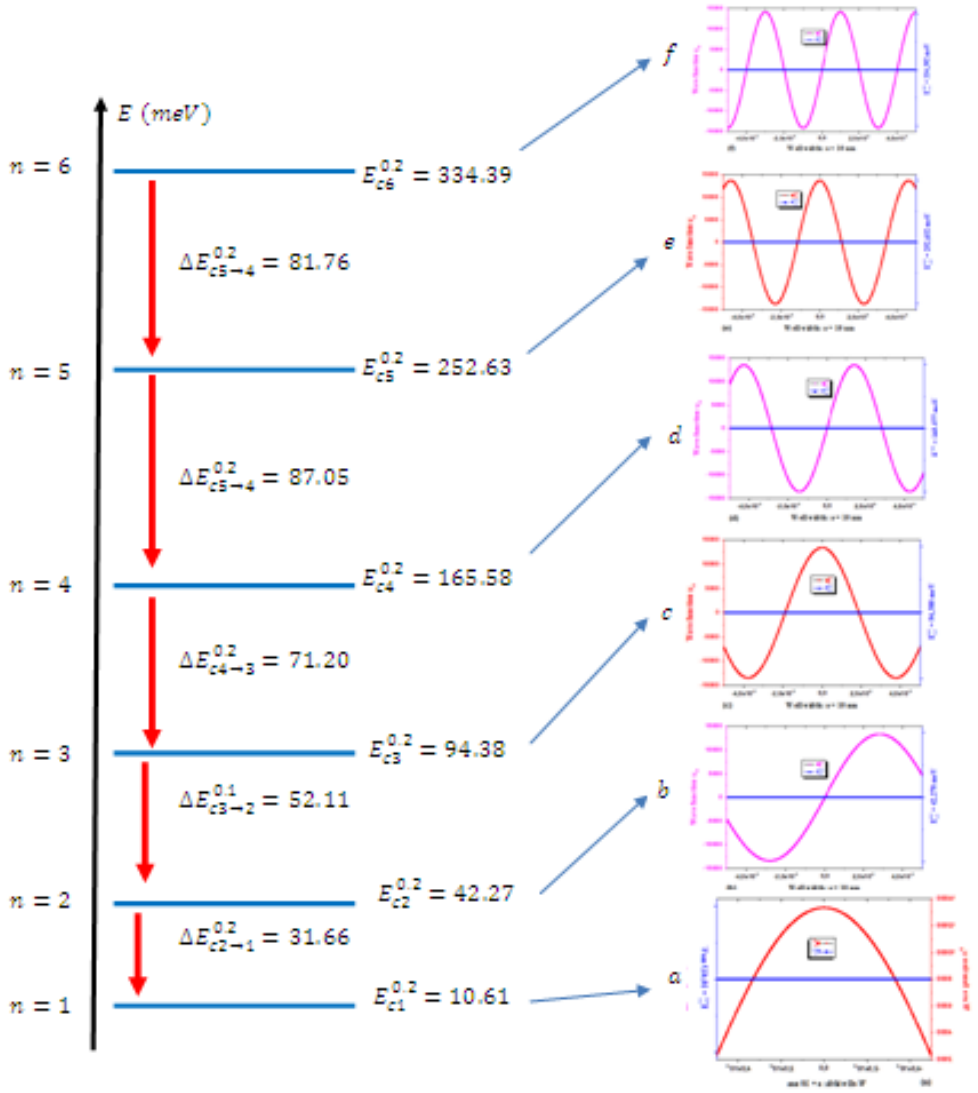

Fig. 4. Energy band diagram for $x = 0.2$ and the associated profiles wave functions $\psi_{II}(z)$ profiles for $x = 0.2$: (a) fundamental level; (b) first excited state; (c) second excited state; (d) third excited state; (e) forth excited state; (f) fifth excited state

Table 1. Solutions for transcendental equations and the related energy levels for electrons in the conduction band for $x = 0.1$, $m^* = 0.28\, m_0$

$k_2 \times 10^8\ (m^{-1})$	2.662	5.269	7.860	10.224
$E\ (meV)$	9.64	38.19	84.11	142.31

Table 2. Solutions for transcendal equations and the related energy levels for electrons in the conduction band for $x = 0.2$, $m^* = 0.28\, m_0$

$k_2 \times 10^8(m^{-1})$	2.792	5.572	8.326	11.028	13.622	15.672
$E\ (meV)$	10.61	42.27	94.38	165.58	252.63	334.39

This case gives six allowed quantum states for electrons in the conduction band, their energy levels and the related wave functions $\psi_{II}(z)$ are represented in figure 4. The wavelengths for the inter level transitions are: $\lambda_{c2\to1}^{0.2} = 39.21\,\mu m$; $\lambda_{c3\to2}^{0.2} = 23.82\,\mu m$; $\lambda_{c4\to3}^{0.2} = 17.43\,\mu m$; $\lambda_{c5\to4}^{0.2} = 14.26\,\mu m$; $\lambda_{c6\to5}^{0.2} = 15.16\,\mu m$. The first two wavelengths are in the far infrared and the last

three ones are in the middle infrared. The photon energy corresponding to the transition between the last excited level and the fundamental one is: $\Delta E_{c6\rightarrow 1}^{0.2} = 323.78\, meV$, corresponding to a wavelength $\lambda_{c6\rightarrow 1}^{0.2} = 3.83\, \mu m$ (middle infrared range). The fundamental state (a) of energy $E_{c1}^{0.2} = 10.61\, meV$, is associated to an even wave function with the amplitude $\psi_{c1_{max}}^{0.2} = 13.35 \times 10^3$. The first excited state (b) ($E_{c2}^{0.2} = 42.27\, meV$) corresponds to an odd wave function with the amplitude $\psi_{c2_{max}}^{0.2} = 13.35 \times 10^3$. The other four excited states (c), (d), (e) et (f) of respective energies $E_{c3}^{0.2} = 94.38\, meV$; $E_{c4}^{0.2} = 165.58\, meV$; $E_{c5}^{0.2} = 252.63\, meV$ and $E_{c6}^{0.2} = 334.39\, meV$, are associated to the alternately even and odd wave functions of amplitudes $\psi_{c3_{max}}^{0.2} = 13.44 \times 10^3$; $\psi_{c4_{max}}^{0.2} = 13.54 \times 10^3$; $\psi_{c5_{max}}^{0.2} = 13.71 \times 10^3$ and $\psi_{c6_{max}}^{0.2} = 14.16 \times 10^3$. For $x = 0.1$, it is noted an increase in the amplitude of the wave function with the excitation and the presence of nodes for the excited states. Just as with the energy levels, for the same quantum number n, the maxima of the wave function are more important for $x = 0.2$.

4. CONCLUSION

The present study, through a graphical resolution of Schrödinger equation, shows that the electrons energy spectrum inside the well in the conduction band of $Zn_{1-x}Mg_xO/ZnO/Zn_{1-x}Mg_xO$ heterostructure is a finite sequence of discrete energy values E_n: $E_1 < E_2 < E_3 \ldots < E_n < V_0$. The work shows that ZnO layer constituting the well, is so thin that the electrons undulatory behavior cannot be neglected. Due to the non-zero value of wave function outside of the well, a non negligible probability exist to find there the electron by “tunneling effect”, a purely quantum phenomenona meaning the existence of evanescent waves. The allowed states in the structure correspond to stationary waves in the direction perpendicular to the layers. Hence, the system is quantized and the quantum confinement effect can be estimated via a simple effective-mass approximation model. The energy of the discrete quantum states depend on the quantum number n and the concentration x of Mg. For a given value of n, the energy increases with x, just as well as intra band transitions between two consecutive levels which augment with n . Consequently, the corresponding infrared wavelengths decrease and also depend on the concentration x. This suggests that it is possible to control the optoelectronic properties of a quantum well by adjusting the concentration during the growth process, in order to obtain the desired wavelength for a semiconductor laser. Many of the physical effects in quantum well structures can be seen at room temperature and can be exploited in real devices like laser diodes, infrared lasers, blue lasers, fiber optic transmitters, infrared photodetectors, high electronic mobility transistors “HEMT” [14, 15].

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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