Theoretical and simulation study of pressure and temperature effect on the electronic states induced by the presence of a material defect in ZnO/ZnMgO MQWs

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Abstract. This work deals with a theoretical study of the effect of pressure and temperature on the electronic states induced by the presence of a material defect in ZnO/$Zn_{1-x}Mg_xO$ Multi-Quantum wells. To determine the transmission coefficient of our structure, we use a mathematical language very well known for composite materials that of the response theory, also called the green function. We demonstrate that the insertion of a material defect in the middle of the MQWs allows our systems to be like symmetrical systems and amplifies the electronic transmission of the defect state. Moreover, we found that the hydrostatic pressure increase induces a noticeable shift of the electronic state towards the lower energies due to the increase of the effective mass. This behavior will be reversed for the increase in the temperature. Our results were validated and compared with those of the literature. The change of position of the defect state allows us to use this structure as a regulable pressure and temperature sensor.

1 Introduction

Due to the exceptional properties (optical and electronic) of the II/VI-III/V semiconductors, and their applications in many areas, such as the fabrication of quantum wells. The fabrication of quantum well based on II/VI-III/V semiconductors was proposed by Esaki and Tsi, as it was used in several fields of application, such solar cells [1], lasers [2], and photodetectors [3]. These quantum wells are composed by two different semiconductors, The first forms the wells and the second forms the barrier. As an example, F. Z. Elamri et al [4-5] studied the behavior of localized states in a GaAs/AlGaAs MQW created by a material or geometrical defect, and found that the physical parameters of the defect (position, concertation, thickness of the defect layer) play a important role in improving the amplitude of the defect state that appears in the gap. Also, the number of localized states appearing in the bandgap is related to the physical parameters of the defect such as a defect position, the molar concentration of Al, and the defect thickness. In addition, M. Kutrowski et al. [6] have studied the luminescence of deep CdTe quantum wells surrounded by $Cd_{1-x}Mn_xTe$ barriers for a concentration variation 0, $1 < x \leq 1$ and a width of the quantum wells varied from 13 A ° to 100 A °. Periodic systems are increasingly used for different applications such as sensors, which are devices that serve to monitor and detect small changes in temperature, pressure, or magnetic field, etc., [7-9] due to their high sensibility. We can find sensors based on photonic structures and multi-quantum well sensors based on semiconductors. For example, we find that Y. Ben-Ali et al. [10] have worked on a pressure and temperature sensor based on a photonic structure consisting of two alternating layers of SiO_2 and TiO_2 with

a GaAs defect layer which has a permeability dependent on pressure and temperature, they have found the appearance of defect states in the band gaps which are sensitive to pressure and temperature variation. In addition, A. Nagaty et al. [11] have studied the propagation of longitudinal acoustic waves in a 1D phononic crystal containing a piezomagnetic material as a defect layer, the results obtained are very useful for the application of this structure as a sensor measuring magnetic fields and for the early detection of cracks in the buildings. The majority of the sensors used are based on the change of the position of peaks that appear in the transmission spectrum due to the introduction of defects inside the structure that break the periodicity, although we find sensors that depend on the change of the intensity of defect peaks. For example, A. Mehaney et al. [12] have presented a sensor to detect CO_2 pollution based on silicon phononic crystal containing rubber layers on both sides of the Phononic crystal to introduce resonance peaks, which help to detect CO_2 gas by changing the intensity of the state. Our main purpose is to study the effect of applying temperature and the pressure on the transmission spectrum through ZnO/ $Zn_{1-x}Mg_xO$ multi-quantum wells structure with a GaN material defect. As a goal we are looking for a good transmission with high-quality factor for a defect state appeared inside the band gap (i.e., small width at half height, and a higher sensitivity with pressure and temperature), which allows us to use this structure as an adjustable pressure or temperature sensor. Our work is structured as follows: in section 1 we begin with a description of the studied structure and some works on the applications of periodic systems. Move on to section 2, which is reserved for the structure parameters like effective mass and gap energy, barrier heights and thicknesses for each material. In section 3, we present and

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discuss the obtained results. Finally, we end this work with a conclusion.

2 Theoretical Statel

The mathematical language we use in this article is that of the response theory, also called the green function, which is used to determine the physical properties of the structure. In our work, we are interested in the transmission coefficient. The general approach of this method is to determine the transmission coefficient from the resolution of the following set of equations [4]:

The cleavage operator $\overleftrightarrow{V}(M_P, M_P)$ is written as follows:

$$\overleftrightarrow{V}(M_p, M_p) = \overleftrightarrow{d}^{-1}(M_n, M_n) - \overleftrightarrow{g}^{-1}(M_n, M_n) \quad (1)$$

The interface response operator $\overleftrightarrow{A}(M_p, M_p)$ is written as follows:

$$\overleftrightarrow{A}(M_p, M_p) = \sum_{M_s} \overleftrightarrow{V}(M_p, M_p) . \overleftrightarrow{g}(M_p, M_p) \quad (2)$$

The operator $\overleftrightarrow{\Delta}(M_p, M_p)$ is written as follows:

$$\overleftrightarrow{\Delta}(M_p, M_p) = I + \overleftrightarrow{A}(M_p, M_p) \quad (3)$$

The Green function of the interface $\overleftrightarrow{d}(M_0, M_0)$:

$$\overleftrightarrow{d}(M_0, M_0) = \overleftrightarrow{g}(M_0, M_0) \overleftrightarrow{\Delta}^{-1}(M_0, M_0) \quad (4)$$

The structure parameters such the thickness of layers can be modified by the applied pressure on the structure

$$d(P) = d_0(1 - (S_{11} + 2S_{12})P) \quad (5)$$

The thickness represents the initial thickness at P= 0 Kbar, are the elastic constates S_{11} and S_{12} are calculated using C_{11}=209, 209+89.x, 390 (×10 Kbar) and C_{12}= 120, 120-24.x,145 (×10 Kbar) respectively for ZnO, $Zn_{1-x}Mg_xO$ and GaN [13-14].
The pressure also modifies the effective masses. For

both the ZnO and GaN wells, the expression is [15]:

$$\frac{m_0}{m_e^*} = 1 + \frac{E_P((Eg(P,T) + \frac{2}{3}\Delta_0))}{(Eg(P,T)((Eg(P,T) + \Delta_0))} + 2F \quad (6)$$

Where, m_0 is the mass of free electrons, Ep is the Kane energy, for ZnO Ep=28.2 eV, 14 eV for GaN [16], [14], Δ_0=0.013 eV for ZnO and 0.014 eV for GaN is the spin-orbit fractionation [13], [14], F is the Kane variable for the ZnO -2.51 and for GaN, it's equal to zero. Eg (P, T) is the gap energy of ZnO and GaN. The expression of E_g (P, T) is [17], [18]:

$$Eg(P,T) = Eg(0.0) + \alpha P - \beta P^2 - \frac{\gamma T^2}{(T+\delta)} \quad (7)$$

Where Eg (0.0) represents the gap energy at P= 0 Kbar and T= 0 K, for the ZnO 3.44 eV and GaN 3.47 eV. For the ZnO and GaN respectively the coefficient α is equal to 0.0024 eV/Kbar and 0.0042 eV/Kbar. In addition, the coefficient β is equal for both materials to 0.2810-5 eV/Kbar2, 1.82810-5 eV/Kbar2. And the temperature coefficient γ, δ of ZnO and GaN, were taken from Ref [18-19].
The effective mass of ZnMgO [13]:

$$m_e^*(Zn_{1-x}Mg_xO) = m_e^*(ZnO) + 0.05.x.m_0 \quad (8)$$

Where x is the concentration of Mg in the barrier layer.

3. Results and discussions

Initially, we consider a periodic perfect ZnO/$Zn_{1-x}Mg_xO$ multi-quantum wells of type I limited by two substrates of the same type ZnO [20] containing 10 cells. The thicknesses of the wells and barrier are respectively equal d_1=d_2=40A°. In the structure of ZnO/$Zn_{1-X} Mg_xO$, the concentration of Magnesium must be x≤0.35 [21] for it to crystallize into the wurtzite structure since this phase is thermodynamically more stable than the cubic phase. For this purpose, we set the magnesium concentration value to 0.25.

Fig. 1. Energetic profile of a MQWs constituting of 10 periods, ZnO/$Zn_{1-X}Mg_xO$ (x = 0.25) with thicknesses equal d_1=d_2= 40A°.
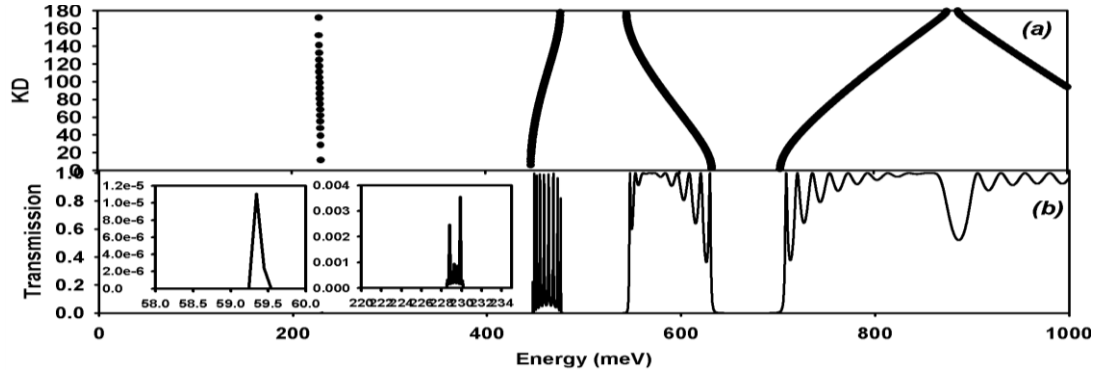

In Fig 2-a, we plot the dispersion relation (KD) as function energy. We observe black branches due to electronic states inside the allowed bands. (Fig.2-b) We also observe that around 230 meV, there is a very narrow allowed band

that cannot be observed in the transmission spectrum (Fig.2-b). This is because its transmission is very small and is of 10-3. Normally, there is another allowed band around 59meV due to the tunneling effect, which has a lower transmission of the order of 10-5. Furthermore, we

determine that no electrons can cross the barrier for [0meV, 59meV] because the barrier's potential energy is higher than that of the incident electrons. Also, we observe in Fig.2-b that bands gaps are separated by the allowed bands. Within these bands, the electrons cannot propagate.

Fig 2. (a)Dispersion curve. (b) Transmission spectrum for a perfect finite structure.

To clarify the behavior of the band structures, we will begin by studying the effect of temperature and pressure on our perfect structure, ZnO/Zn$_{1-x}$Mg$_x$O. In fig.3-a, we examine the effect of pressure on the transmission spectrum at a fixed temperature of 300K for different pressure values P= 0 Kbar (black), P= 5 Kbar (red), P=10 Kbar (blue). We can notice that the permissible bands shift towards the lower energies when the pressure increases, which is similar to the results found in [22]. According to these results, we can also notice that for a pressure range between [0 Kbar-10 Kbar], the shift of the transmission spectrum has a little variation with the pressure, and whenever we make a variation of 5 kbar, the pass bands move about 2 mev towards the lower energies. In fig.3-b, we evaluate the impact of the temperature variation from [0 K-300 K] on the transmission spectrum for a fixed pressure of 0 Kbar. We notice that the temperature increase induces a noticeable shift of the bands towards higher energies, contrary to the variation of the pressure. In Fig 4-a, b, we examine the effect of pressure and temperature on the effective mass of ZnO and ZnMgO. We can determine that the pressure and effective mass are proportional, which implies that increasing the pressure induces a decrease in electron mobility in our structure, which prevents the allowed bands from moving to low energies upon increasing the pressure.

On the other hand, we also notice that the impact of temperature on the effective mass is reversed compared to pressure. This allows us to conclude that the temperature and the effective mass are inversely proportional, so the increase in temperature induces an increase in the mobility of electrons. These external perturbation effects allow us to adjust or control the movement of the bands to higher or lower energies.

Fig 3. (a) Electron transmission spectrum for varied pressure values [0 Kbar-10 Kbar] at T = 300 K. (b) For varied temperature values [0 K-300 K] at P = 0 Kbar.
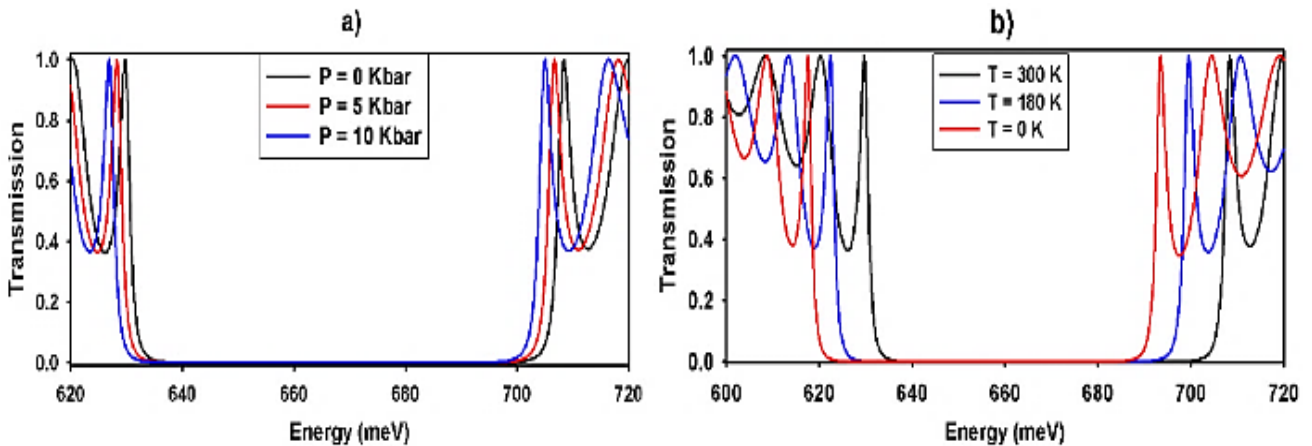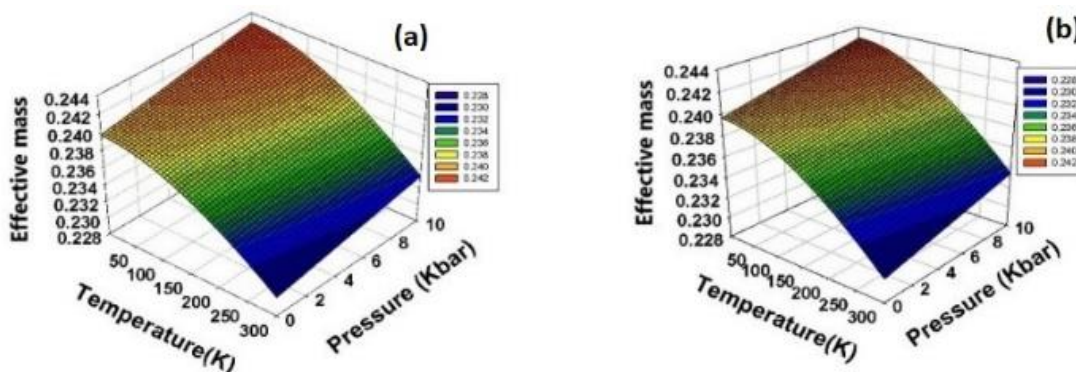
Fig 4. Variation of the effective mass as a function of pressure and temperature, (a) for ZnO and (b) for ZnMgO.

In the second part, we considered multi-quantum wells with a defect layer GaN of a thickness $d_0=35A°$ located in the structure's middle ($J_{def} = 5$). The figure below (Fig.5) describes the structure used in our study. The parameters of the defect are given in Table 1. In Fig.6, we present the transmittance spectrum at a pressure value $P = 0$ Kbar and a temperature equal to 300K. It is found that there are defects states within the band gaps that correspond to localized states that favor electron transport. In the range of [470 meV-550 meV], there is an appearance of a defect state with transmission about 0.58, closer to the passband. On the other side, we can see the presence of a very narrow peak around an energy of 670 meV with a transmission equal to 0.96 in the energy interval [610 meV-715 meV]. In the following, we examine the effect of pressure and temperature on the defect states that appear in Fig.6 to determine our structure's sensitivity with the variation of these external disturbances. We are particularly interested in the peak in the [610 meV-715 meV] interval, which has a strong transmission, localized in the middle of the bandgap. Fig.7-a represents the variation of transmission coefficient as a function of pressure and the energy for a defect state that occurs in the [610 meV-715 meV] interval. As the pressure increases, this state shifts towards lower energies, which is due to the decrease in electron mobility. Furthermore, we discovered that applying pressure on our structure changes the transmission of the defective state. On the

other hand, we plotted the transmission spectrum (Fig.7-b) as a function of the incident electrons energy (0 Kbar, 5 Kbar, and 10 Kbar) for various pressures. This helps us to determine the quality for transmission peak, with Q is the ration of the central energy of the peak and the maximum width at half-maximum of the energy. The electronic state moves towards lower energies while the quality factor Q increase as a function of the increasing pressure, shown in Table 1. In contrast to the results obtained in Fig 7, we have now fixed the pressure at 0 Kbar while varying the temperature between 0 and 300K. We find that as the temperature increases, the defect state shifts to higher energies (Fig.8-a) because of the increase in electron mobility. Thus, we plotted the transmittance spectrum for different temperature values in order to define the sensitivity of the electronic state while varying temperature (Fig.8-b). For temperatures below 20 K, the states are superimposed on each other, but if we increase the step to 20 K, we can notice distinct defect states. We can conclude that for a temperature variation of T = 20 K, our structure will detect a significant change in the central energy of the defect states. Furthermore, the quality factor Q of the defect state can be determined from the representation of the electronic transmission spectrum (Fig.8-b), which allows us to conclude that the quality factor of the electronic state decreases, with a shift to higher energies as shown in Table 2.

Fig. 5. MQWs structure with a material defect GaN in the middle ($J_{def}= 5$), the whole structure is sandwiched between two substrates
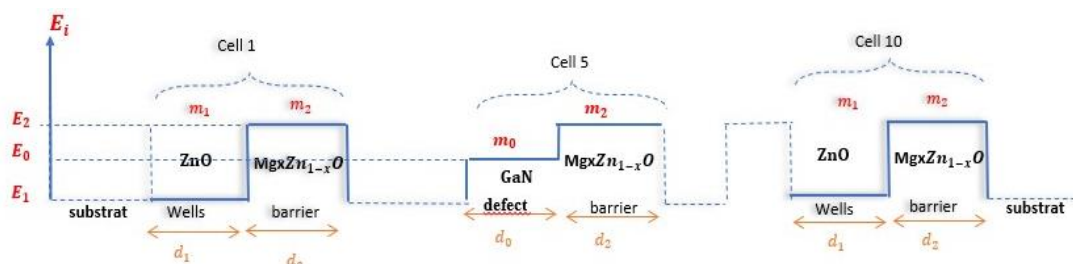
Fig 6: Transmission spectrum versus energy for an MQWs with a defective layer
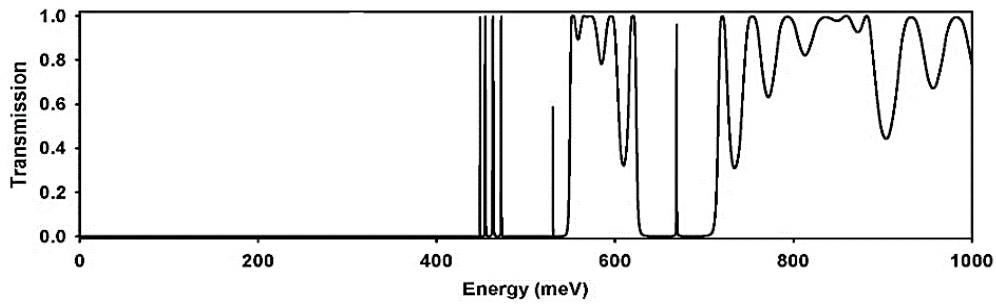

Fig 7: (a) Transmission spectrum of hydrostatic pressure and energy. (b)Transmission spectrum versus energy for an MQWs with a defective layer for varied pressure values [0 Kbar-10 Kbar] at T = 300 K.
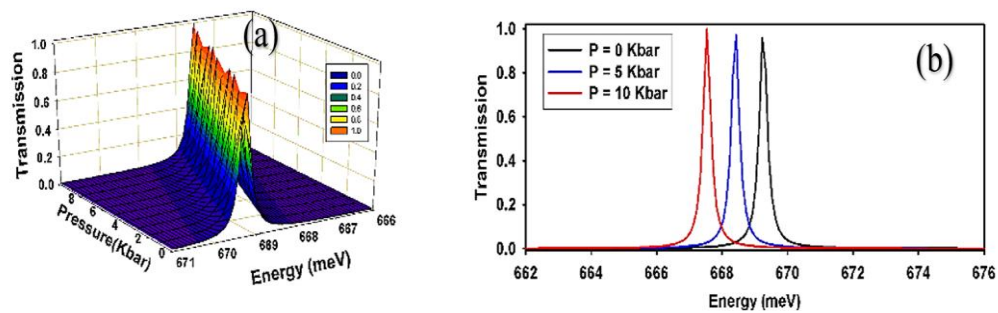

Table 1: Quality factor for pressure interval of [0 Kbar- 10 Kbar].

Pressure	0 Kbar	5 Kbar	10 Kbar
Quality Factor	3042.68	3342.64	4172.56

Fig 8: (a) Transmission spectrum of the temperature and the energy. (b) Transmission spectrum versus the energy for an MQWs with a defective layer for different temperature values.
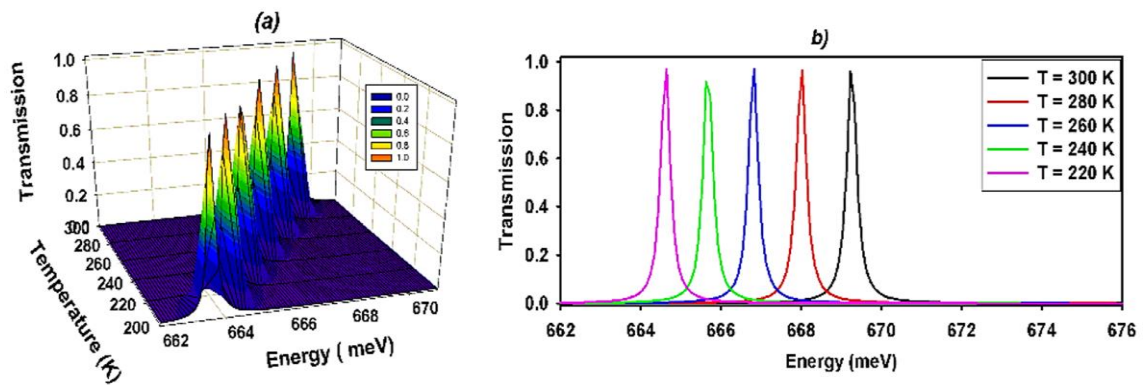

Table 2: Quality factor for temperature interval of [220 K- 300 K].

Temperature	220 K	240 K	260 K	280 K	300 K
Quality Factor	4154.56	3740.241	3704.788	3514.57	3042.68

4 Conclusion

This work represents a theoretical and simulation study of pressure and temperature on MQWs perturbed by a GaN material defect located in the middle of the studied structure, which allows us to realize a symmetric system. We investigated the possibility of using our structure, which contains a material defect GaN, as a controllable pressure or temperature sensor. We found that the introduction of a defect in the perfect periodic structure ZnO/$Zn_{1-X}Mg_xO$ induces defect states in the band gaps, which are sensitive to external perturbations (pressure and temperature), such that an increase in pressure shifts them to lower energies, while an increase in temperature shifts them to higher energies. Furthermore, we found that these perturbations influence the transmittance of these states and their quality factors. In our study, we found for a step size of $\Delta T=20$ K and $\Delta P=5$ Kbar, we have defect states that are distinct from each other. Therefore, we can conclude from these results that our structure can be used as a pressure or temperature sensor based on the displacement of the defect states that appear in the band gap.

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