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Electronic and Optical Properties of GaN / AlN Multiple Quantum Wells under Static External Magnetic Field

M. Solaimani, M. Izadifard

Faculty of Physics, Shahrood University of Technology, Shahrood, Iran

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In this work, we have investigated the effect of an external magnetic field and, for the first time, number of wells with constant total effective length to study the degeneracy in electronic energy levels. We have used constant total effective length because it is technologically important. Then we have tried to remove the n-fold degeneracy of the n-well multiple quantum well by means of the external magnetic field but the two-fold degeneracy was remain and not removed. Finally, the effect of the external magnetic field on the number of bound states and the situation of unchanging absorption coefficient in a wide magnetic field interval are also investigated.

Keywords: Electronic energy levels, Magnetic field, Single and multiple quantum wells, Finite difference method, Linear absorption coefficient.

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1. INTRODUCTION

Semiconductor nanostructure systems like quantum wells have an essential role in the modern nanotechnologies. Based on this importance, a great amount of investigations have devoted to this field of study. In this way, different geometrical shapes of the quantum well systems have been investigated. Some of these shapes are: hyperbolic quantum well [1], triangular quantum wells [2-3], delta-doped quantum well [4], and some others [5]. Besides, the effect of wells number in double quantum well [6-7] and triple quantum well [8] have also been studied. Magnetic field is also a flexible tool to modify or change different properties of these systems. The magnetic field changes the confinement potential, then the electronic structure of the system will be modified.

Here we have used another interesting way to construct our quantum confinement geometry which we expect find good situation in the modern technologies. Retaining the total length of the structure constant and varying the number of wells within it in our resent studies [9-10], led to Constant Total Effective Length Multiple Quantum Wells (CTEL-MQWs). Our strategy of building multiple quantum wells may lead to smaller nano-devices with optimized physical properties and at the same time we have saved the time and material needed to fabricate the device. Since, one of the most challenging parameters in modern technologies is the device size, Here, by tuning the total effective length of the structure, smaller devices may be fabricated. In the present work, we have tried to study the effect of the number of wells on energy levels of a GaN / AlN MQW system with constant total effective length and same well and barrier thicknesses. The effect of the applied magnetic field on the ground state wave function and energy levels and the degeneracy in them, number of bound states and also the effect of the magnetic field on the linear absorption peak positions are investigated. Finally, we have used a Finite Difference method to solve our Schrödinger Hamiltonian.

2. FORMALISM

The effective Schrödinger equation in the effective mass approximation and within the envelop function method in the presence of an external magnetic field perpendicular to the growth direction is [11],

$$H\psi(x)=\left(-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2}+\frac{e^2B^2x^2}{2m^*c^2}+V(x)\right)\psi(x)=E\psi(x) \qquad (1)$$

Where m^* is the effective mass, c is the speed of light in free space, e is the electron charge and B is the applied external magnetic field perpendicular to the growth direction. The eigen-energies and eigen-function have been investigated by the numerical discretization methods[12]. Then the first order absorption coefficient $\alpha^{(1)}(\omega)$ for intersubband can be calculated by [13],

$$\alpha^{(1)}(\omega)=\frac{\omega\mu c}{n_r}\left|M_{fi}\right|^2\frac{m^*k_BT}{L_{eff}\pi\hbar^2}\ln\left[\frac{1+\exp\ (E_F-E_i)/k_BT}{1+\exp\ (E_F-E_f)/k_BT}\right] \times\frac{\hbar/\tau_{in}}{(E_f-E_i+\hbar\omega)^2+(\hbar/\tau_{in})^2} \qquad (2)$$

where ω is the angular frequency of the excitation electromagnetic field, E_F represents the Fermi energy, E_i and E_f denote the quantized energy levels for the initial and final states, respectively, k_B is the Boltzmann constant, c is the free space speed of light, L_{eff} is the effective spatial extent of electrons, n_r is the refractive index, τ_{in} is the intersubband relaxation time (which we have used the numerical value of 0.14 ps [14]). Moreover in these equations M_{fi} is the dipole matrix element which is defined as [13],

$$M_{fi}=\int\varphi_f^*(z)\,|e|\,z\varphi_i(z)dz \qquad (3)$$

In order to evaluate the Fermi energy we have used the 2D-electron density,

$$n^{2D} = \sum_{j=1}^{n} n_j^{2D} = \frac{m^* k_B T}{\pi\hbar^2}\sum_{j=1}^{n}\ln(1+\exp((E_F-E_j)/k_BT)) \quad (4)$$

which was taken from [15]. In this equation j represents the subband state number. In order to find the Fermi Energy we have used the $n^{2D} = 3.0 \times 10^{16}$ [14] and then by varying the Fermi energy we have tried to find the true EF.

3. RESULTS AND DISCUSSION

In this work we have applied an external magnetic field perpendicular to the growth direction of a GaN / AlN MQWs structure including of 1 to 7 numbers of wells. For this purpose, we have used $m^* = 0.15\ m_0$ (where m_0 is the free electron mass), the barrier height $V_{conf} = 1.28$ eV [15], $L_{eff} = 600$ Å. In our calculations we have used equally spaced wells in a MQWs with the same well and barrier widths. For example in a triple quantum well we have three wells with well width of (600 / (3 + 4)) Å. Thus the well width for a MQW with n wells can be found by (600 / (2n + 1)) Å.

In the Fig. 1 we have tried shown the subband energies versus an external magnetic field B perpendicular to the growth direction for MQWs ($1 \le n \le 6$). In parts 2 (a-f) two, three, four, five and six lowest states for these MQWs have been shown and within the inset the sixteen lowest subband is presented.

The insets is presented to find out that the intersection of subband will be occurred or not and of course for more illustrations. The n-fold degeneracy at $B = 0$ is clearly from these figures. By increasing of the well number $n > 2$ and the magnetic field some degeneracy

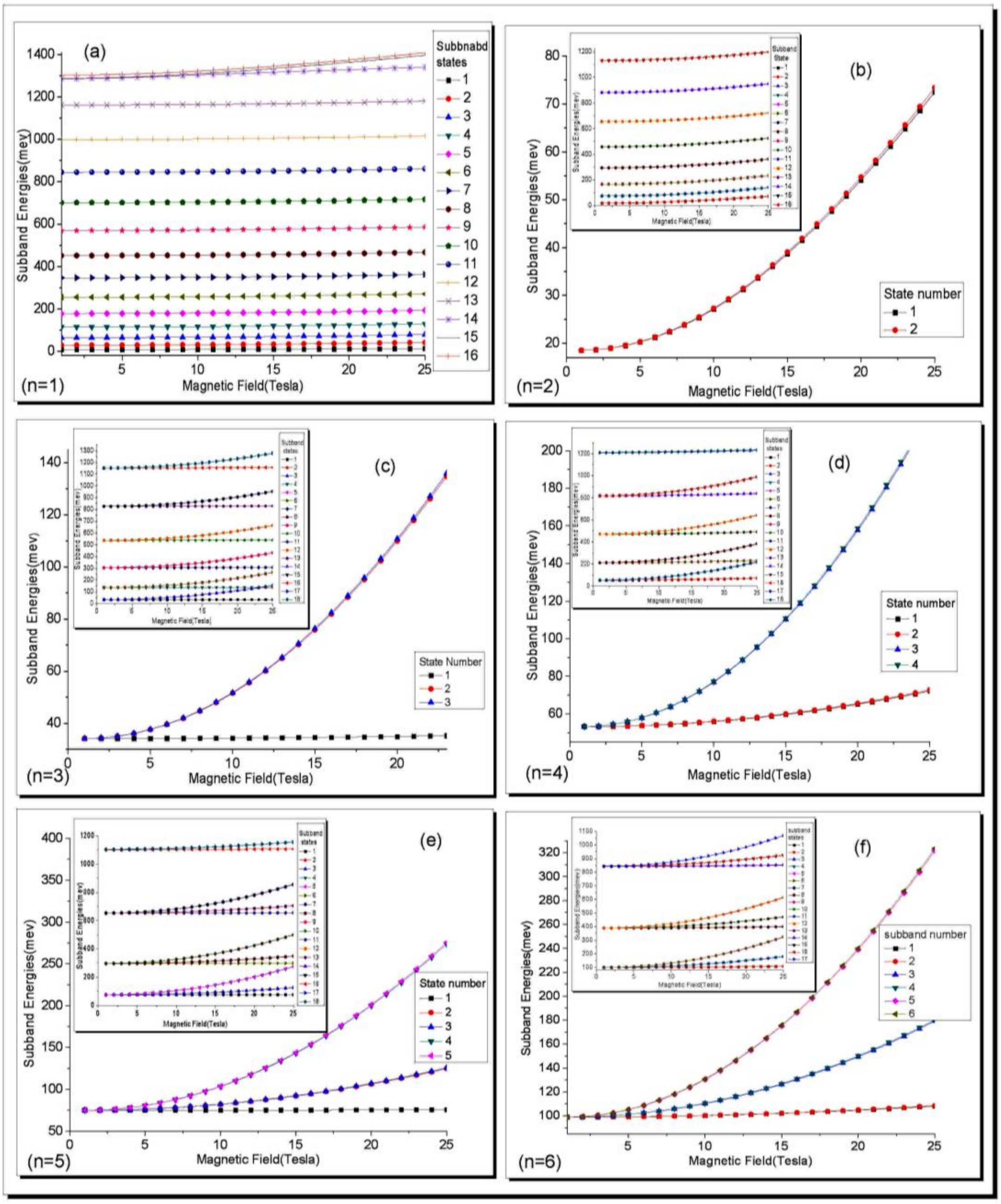

Fig. 1 – Effect of an external magnetic field B perpendicular to the growth direction on subband energies of some MQWs with different number of wells

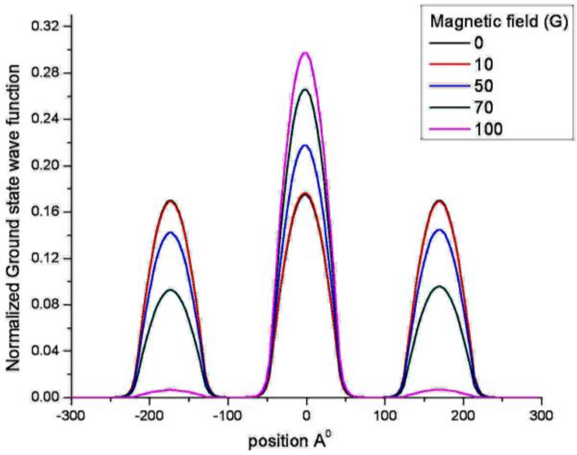

Fig. 2 – Effect of the magnetic field on the ground state wave function of a 3-well MQW

are removed. For double quantum well by increasing of the applied magnetic field the degeneracy is almost remains. For MQWs with an odd number of wells the ground state is not degenerate but for MQWs with even well numbers we have two fold degenerate states. For example in the 3-well MQWs the ground state has not degeneracy in the presence of the magnetic field but the first excited state has two-fold degeneracy. But for 4-well MQWs both ground and excited states have two fold degenerate states. This behavior is also seen by calculating of other excited states (inset figures). In general the magnetic field can split the n-fold degenerate subband of an n-well MQWs (n = even and $B = 0$ T) into $n / 2$ two fold degenerate subbands. The intersection of the subband energies in the presence of the external magnetic field (about 25 T) will take place for MQWs with $n > 2$. The underplaying reason for the de-

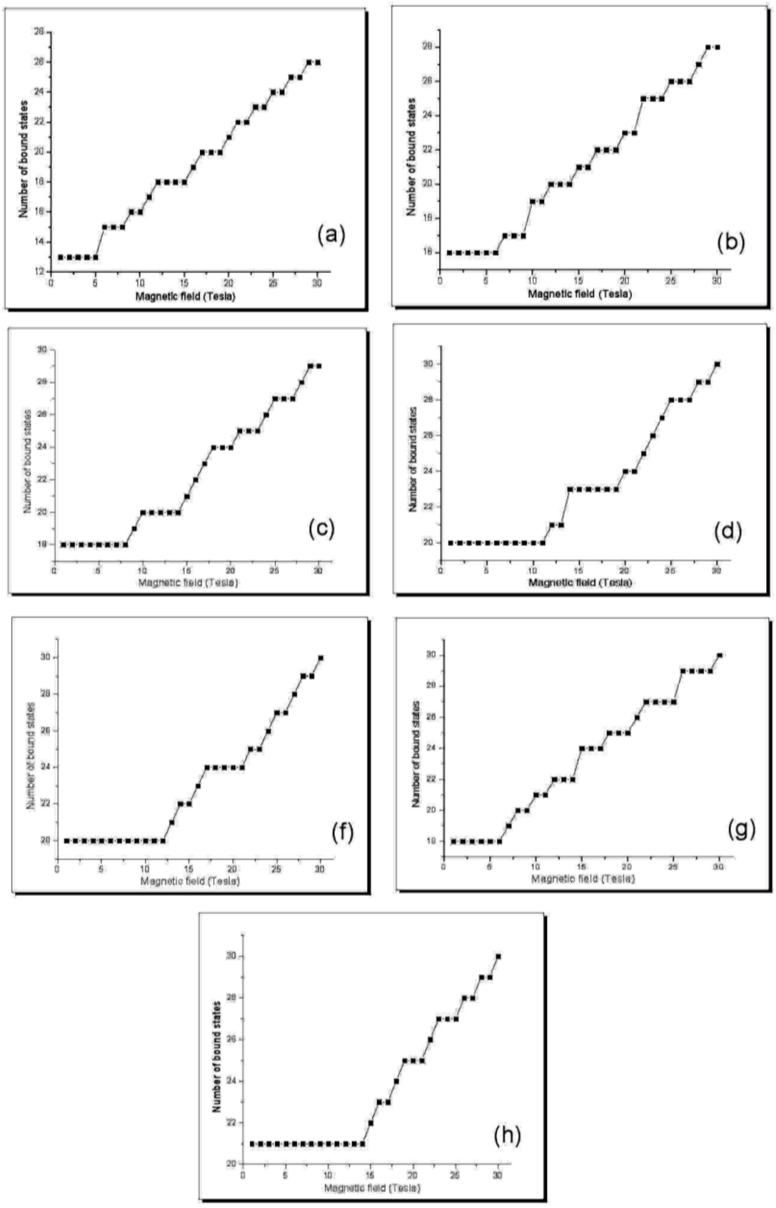

Fig. 3 – Effect of an external magnetic field B and number of wells on the number of bound states of the quantum system

generacy removal property of the external magnetic field is that, the magnetic field adds a parabolic term to the confinement potential and thus magnetic field changes it. Now the existing wells in a multiple quantum well have not exactly the same geometrical shape and thus the energy levels are not degenerate like prior to the application of the magnetic field (as we know, a multiple quantum well with n identical wells the wells have n-fold degeneracy[10]). But the parabolic potential which magnetic field adds is a symmetric potential with respect to the centre of the central well. Now $n/2$ of the wells have same geometrical shape as the other $n/2$ wells thus the magnetic field splits the n-fold degenerate subband of an n-well MQWs ($n =$ even and $B = 0$ T) into $n/2$ two fold degenerate subbands.

In the Fig. 2 we have presented the effect of the magnetic field on the normalized ground state wave functions of MQWs including of 3 wells.

This figure show that at zero magnetic field there 3 peak which are localized within three wells. As it can be seen the central well is slightly more probable to include the electron. Increasing of the magnetic field up to 100 G leads to the localization of the wave function within the central well. It could be due to the fact that the external magnetic field adds a parabolic term around the origin to the potential of the system.

In the Fig. 3 we have presented the effect of an external magnetic field B and number of wells on the number of bound states of our quantum systems. In all of these systems, increasing of the external magnetic field enhanced the number of bound states. But as it is clear from the figure it increased in a stepwise manner. This can be expected from the fact that the energy levels of a quantum system are discretized. When we increase the amount of the external magnetic field (and thus the confinement of the free carriers), then in some special values of the external magnetic field a new energy level fall within the bound states region. Thus in this interval of the magnetic field the number of bound states remain constant. On the other hand, at zero magnetic field, the larger the number of wells can the more number of bound states. In the meantime in some special number of wells there is a rather wide magnetic field interval within which the numbers of bound states do not change. This has direct effect of the optical properties on the system like absorption coefficient we have presented in the next figure.

In the Fig. 4 we have presented the effect of an external magnetic field B and incident photon energy on the linear absorption coefficient of our quantum systems. Each point the plot is the absorption peak position which occurred in a special incident photon energy and external magnetic field.

As we can see in this figure, increasing of the external magnetic field leads to the peak positions which occur in the greater incident photon energy. If we put aside the single quantum well, then the slop of the diagram decreases by increasing of the number of wells. As we saw in the previous figure, in some special number of wells there was a rather wide magnetic field interval within which the numbers of bound states did not changed. The systems which had wider unchanging magnetic field interval in the number of bound state diagram, now have wider magnetic field interval within which the apportion peak position do not change.

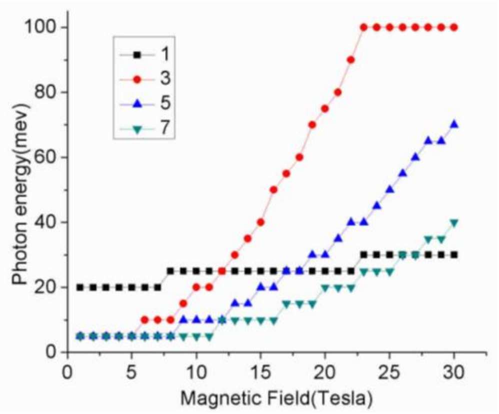

Fig. 4 – Effect of an external magnetic field B and incident photon energy on the linear absorption coefficient of the quantum system

If we need a system which we like to have unchanging absorption coefficient in a wide magnetic field interval we have to use multiple quantum wells with greater number of wells.

4. CONCLUSION

In this study, the effect of external magnetic field and number of wells on the electronic structure and optical properties MQWs is investigated. In the n-well MQWs with number of wells greater than 6, the n-fold degeneracy is not seen and we had a supperlattice. Thus the splitting of the subbands was not so large which is due to the depth of the well which is approximately high. It tried to remove the degeneracy of the n-well MQWs ($2 \leq n \leq 6$) by an external magnetic field B perpendicular to the growth direction. The degenerate states split into some 2-fold degenerate states. Increasing of the external magnetic field enhanced the number of bound states. In some special number of wells there was a rather wide magnetic field interval within which the numbers of bound states did not change. Increasing of the external magnetic field led to the peak positions which occurred in the greater incident photon energy. If we need a system which we like to have unchanging absorption coefficient in a wide magnetic field interval we had to use multiple quantum wells with greater number of wells.

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