# Temperature dependence of width band gap in $In_xga_{1\text{-}X}as$ quantum well in presence of transverse strong magnetic field

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**Abstract.** This article investigated the temperature dependence of the width band gap in $In_xGa_{1-x}As$ quantum well in the presence of a transverse strong magnetic field. A new method was proposed for determining the width band gap of $GaAs/In_xGa_{1-x}As$ heterostructures based on a $In_xGa_{1-x}As$ quantum well in the presence of a magnetic field and temperature. An analytical expression is obtained for calculating the width band gap of a rectangular quantum well at various magnetic fields and temperatures.

## 1 Introduction

Currently, research is being carried out on photo and magnetic quantum effects (properties) in quantum-dimensional heterostructure materials [1,2]. The study of oscillations of the density of energy states in the allowed zone of the quantum well, in particular, under the influence of temperature and a strong magnetic field, reveals new physical aspects of this direction [3-5]. In particular, the study of the effect of a quantizing magnetic field on oscillations of the density of states leads to radical changes in the conduction and valence bands of the quantum well. In such experiments, as a rule, the oscillations of the density of states in the allowed band of the quantum well, the effective mass of charge carriers, the magnetic susceptibility oscillations, and the magnetoresistance oscillations are determined [6-11]. The temperature dependence of discrete Landau levels of charge carriers in the conduction band and the valence band of quantum-well heterostructures can be used to study the temperature dependence of the band gap of a quantum well under the action of a transverse quantizing magnetic field. In massive and low-dimensional semiconductor structures, controlling the band gap under the influence of external fields is one of the urgent problems in creating various micro, nano, and optoelectronic devices. However, until now, no theory has been developed with the help of which it would be possible to specifically determine the width of the forbidden zone of the quantum well for different temperatures and in the presence of a transverse quantizing magnetic field.

In recent years, the world has been increasingly interested in studying the problem of creating devices for micro, nano, and optoelectronics, the main elements of which will be heterostructures based on quantum wells [12, 13]. The energy spectrum of electrons and holes in a quantum well's conduction and valence bands is the most important characteristic

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of quantum-dimensional heterostructures [14-17]. The effect of a transverse quantizing magnetic field on the energy spectrum of charge carriers in the allowed band of quantum-well heterostructures has hardly been studied. And theoretical explanations of the cases under the influence of both a transverse quantizing magnetic field and temperature are completely absent. Hence, to develop a new mathematical model, there was an attempt to solve this problem. Following the posed problem, it was necessary to solve the following tasks:

1. Calculation of the temperature dependence of the energy spectrum of electrons and holes in the allowed zone of a rectangular quantum well under the influence of a transverse quantizing magnetic field.
2. Study of the effect of a transverse quantizing magnetic field on the temperature dependence of the band gap of quantum wells with a parabolic dispersion law.
3. Develop a new model to determine the effect of a strong transverse magnetic field and temperature on the band gap of a quantum well.

## 2 Models and methods

In the absence of a transverse quantizing magnetic field, the energy spectrum of charge carriers in the allowed zone of the quantum well $E_n^e, E_n^h$ and the envelope wave function for electrons and holes $\chi_n^e, \chi_n^h$ are easily found from the one-electron Schrödinger equation [1, 2]:

$$\begin{cases} \left(-\dfrac{\hbar^2}{2m_e}\dfrac{\partial^2}{\partial z^2}+E_c(\mathrm{z})\right)\chi_n^e(\mathrm{z})=E_n^e\chi_n^e(\mathrm{z}) \\ \left(\dfrac{\hbar^2}{2m_h}\dfrac{\partial^2}{\partial z^2}+E_V(\mathrm{z})\right)\chi_n^h(\mathrm{z})=E_n^h\chi_n^h(\mathrm{z}) \end{cases} \tag{1}$$

Here, $m_e$, $m_h$ are effective masses of electrons and holes. $E_c$, $E_V$ is the edge of the conduction and valence bands of the quantum well, and $E_c(z)$, $E_V(z)$ are functions describing the profile of the quantum well. The movement of charge carriers in the conduction and valence bands of the quantum well along the *XY* plane remains unlimited, or the energy spectrum of electrons and holes in such a plane will be quasi-continuous. But, the movement of electrons and holes along the *Z*-axis will be quantized. Hence, the parabolic law of dispersion of the total energy of electrons and holes in the allowed zone of the quantum well has the following form:

$$\begin{cases} E_e\left(E_c,k_e,\mathrm{d},\mathrm{n}_e\right)=E_c+\dfrac{\hbar^2}{2m_e}\left(k_{ex}^2+k_{ey}^2\right)+\dfrac{\hbar^2\pi^2}{2m_ed^2}n_e^2 \\ E_p\left(E_V,k_h,\mathrm{d},\mathrm{n}_h\right)=E_V-\dfrac{\hbar^2}{2m_h}\left(k_{hx}^2+k_{hy}^2\right)-\dfrac{\hbar^2\pi^2}{2m_hd^2}n_h^2 \end{cases} \tag{2}$$

Let us now consider the temperature dependence of discrete Landau levels of electrons and holes in the conduction and valence bands of the quantum well. Transverse quantizing magnetic fields affect the energy spectrum of charge carriers in the allowed zone of a rectangular quantum well. This effect leads to serious changes in the edges of the conduction and valence bands of the quantum well, which is reflected in the oscillations of the density of energy states. In this case, the movement of charge carriers in the valence band and the conduction band of the quantum well along the *XY* plane becomes limited, and the energy of charge carriers in this direction is quantized. Hence, in a transverse quantizing magnetic field, the energy of free charge carriers in the allowed zone of the quantum well, without taking into account the spin, can be written:

$$\begin{cases} E_{e}^{2d}\left(E_c,\omega_c^e,\mathrm{d},\mathrm{n}_e\right)=E_c+\hbar\omega_c^e\left(N_L^e+\frac{1}{2}\right)+\frac{\hbar^2\pi^2}{2m_e d^2}n_e^2 \\ E_{p}^{2d}\left(E_V,\omega_c^h,\mathrm{d},\mathrm{n}_h\right)=E_V-\hbar\omega_c^h\left(N_L^h+\frac{1}{2}\right)-\frac{\hbar^2\pi^2}{2m_h d^2}n_h^2 \end{cases} \quad \text{……..(3)}$$

Here, $N_L^e$ and $N_L^h$ are the number of Landau levels of electrons and holes in the conduction band and in the valence band of the quantum well. Oscillations of the density of energy states in a quantum well's conduction and valence bands, per unit energy range, is an essential characteristic of low-dimensional semiconductor materials. In particular, a change in the energy spectrum of charge carriers leads to a change in the oscillations of the density of states in the allowed bands under the action of a quantizing magnetic field.

In the presence of a transverse quantizing magnetic field, the temperature dependence of the oscillations of the density of energy states can be used to study the temperature dependence of the band gap of the quantum well. We expand the oscillations of the density of energy states of a quantum well, including the conduction and valence bands, in a series using formula (3).

For the conduction band of the quantum well:

$$N_{S,Z}^{c,2d}\left(E,B,T,d\right)=\sum_{N_L,N_e}^{\infty}\frac{eB}{\pi\hbar}\cdot\frac{1}{kT}\cdot\exp\left(-\frac{\left(E-\left(E_c+\hbar\omega_c^e\left(N_L^e+\frac{1}{2}\right)+\frac{\hbar^2\pi^2}{2m_e d^2}N_e^2\right)\right)^2}{\left(kT\right)^2}\right) \quad (4)$$

For the valence band of the quantum well:

$$N_{S,Z}^{\mathrm{V},2d}\left(E,B,T,d\right)=\sum_{N_L,N_h}^{\infty}\frac{eB}{\pi\hbar}\cdot\frac{1}{kT}\cdot\exp\left(-\frac{\left(E-\left(E_V-\hbar\omega_c^h\left(N_L^h+\frac{1}{2}\right)-\frac{\hbar^2\pi^2}{2m_h d^2}N_h^2\right)\right)^2}{\left(kT\right)^2}\right) \quad (5)$$

Expression (3) shows the dependences of the energy of charge carriers on the transverse quantizing magnetic field and on the thickness of a quantum well with a parabolic dispersion law. This energy spectrum is fundamentally altered in the dimensions of a quantum well and a strong quantizing magnetic field. The motion of free electrons and holes in the XY plane becomes quantized, while the motion along Z remains discrete. Hence, it can be seen that under the influence of a transverse quantizing magnetic field, the valence band and the conduction band of the quantum well split into several zerodimensional subbands. In addition, using expressions $E_c(T)-E_v(T)=E_g(T)$ and formula (2), it is possible to calculate the value of the band gap of a quantum well under the action of a magnetic field:

$$\begin{aligned}
&E_g(B,d)=E^{2d}_e\left(E_c,\omega_c^e,\mathrm{d},\mathrm{n}_e\right)-E^{2d}_p\left(E_V,\omega_c^h,\mathrm{d},\mathrm{n}_h\right)\\
&E_g(B,d)=E_c+\hbar\omega_c^e\left(N_L^e+\frac{1}{2}\right)+\frac{\hbar^2\pi^2}{2m_ed^2}n_e^2-\left(E_V-\hbar\omega_c^h\left(N_L^h+\frac{1}{2}\right)-\frac{\hbar^2\pi^2}{2m_hd^2}n_h^2\right)\\
&E_g(B,d)=E_c-E_V+\left(\hbar\omega_c^e\left(N_L^e+\frac{1}{2}\right)+\hbar\omega_c^h\left(N_L^h+\frac{1}{2}\right)\right)+\left(\frac{\hbar^2\pi^2}{2m_ed^2}n_e^2+\frac{\hbar^2\pi^2}{2m_hd^2}n_h^2\right)\\
&E_g(B,d)=E_g(T=0)+\left(\hbar\omega_c^e\left(N_L^e+\frac{1}{2}\right)+\hbar\omega_c^h\left(N_L^h+\frac{1}{2}\right)\right)+\left(\frac{\hbar^2\pi^2}{2m_ed^2}n_e^2+\frac{\hbar^2\pi^2}{2m_hd^2}n_h^2\right)
\end{aligned} \tag{6}$$

Using the formula above, we will also derive the formula for the temperature dependence. To do this, we will use Varsh's empirical expression [18, 19]:

$$E_g(T)=E_g(0)-\frac{\alpha_1T^2}{\alpha_2+T} \tag{7}$$

Hence, substituting (7) into (6), we obtain the effect of a transverse quantizing magnetic field on the temperature dependence of the band gap of a quantum well with a parabolic dispersion law:

$$E^{0d}_g(B,\mathrm{T},d)=E_g(0)-\frac{\alpha_1T^2}{\alpha_2+T}+\left(\hbar\omega_c^e\left(N_L^e+\frac{1}{2}\right)+\hbar\omega_c^h\left(N_L^h+\frac{1}{2}\right)\right)+\left(\frac{\hbar^2\pi^2}{2m_ed^2}n_e^2+\frac{\hbar^2\pi^2}{2m_hd^2}n_h^2\right) \tag{8}$$

## 3 Results and Discussion

Let us analyze the temperature dependence of the oscillations of the density of energy states of specific quantum-dimensional heterostructure materials in a transverse quantizing magnetic field. Fig.1 shows the energy diagram of a $GaAs/In_xGa_{1-x}As$ quantum-well heterostructure with one quantum well exposed to a transverse quantizing magnetic field. The thickness of the quantum well of the $In_xGa_{1-x}As$ solid solution will be in the range $d$ = 1–10 nm, which is much less than the width of the *GaAs* layers (~ 1 μm) [1,2]. The band gap of *GaAs* (*Eg0* = 1.426 eV) is greater than the band gap of the $In_xGa_{1-x}As$ solid solution (*Eg0* = 0.35 eV), and a heterojunction of the so-called "enclosing" type (of the first kind according to another classification) forms at the interface of these materials (Fig.1). In the direction of the *Z* axis - the movement of charge carriers is limited. In the presence of a transverse quantizing magnetic field (B ∥ Z) perpendicular to the *XY* plane, the motion of free electrons and holes is also quantized. Hence, the movement of charge carriers in all directions will be fixed, which is called a quantum dot. The question arises, how to determine the oscillations of the density of energy states for these physical processes, and how temperature affects them? Using the presented new model, it is possible to calculate the temperature dependence of the oscillations of the density of energy states in the conduction band and the valence band of the quantum well of the $In_xGa_{1-x}As$ solid solution. Figure 2 shows the curves of oscillations of the energy density of states in the allowed band of the quantum well of the $In_xGa_{1-x}As$ solid solution at low constant temperatures and at transverse quantizing magnetic fields. Here, B = 10 T, d = 6 nm, T = 5 K, and Eg0 = 0.75 eV. As can be seen from these figures, the conduction and valence bands of the quantum well of the $In_xGa_{1-x}As$ solid solution consist of densely spaced discrete Landau levels of electrons and holes. In the absence of a transverse quantizing magnetic field and at a temperature of T = 5K, the density of energy states in the conduction band and in the valence band of the quantum well of the $In_xGa_{1-x}As$ solid solution is constant $Nss = 4 \cdot 10^{15} eV^{-1}cm^{-2}$, and the band gap is $E_g^{2d}(0) = 0,75\,eV$ (Fig.2). But, if one acts with a transverse quantizing magnetic field (B = 10 T), then the bottom of the conduction band and the top of the valence band move. Then, the band gap of the quantum well of the $In_xGa_{1-x}As$ solid solution increases.

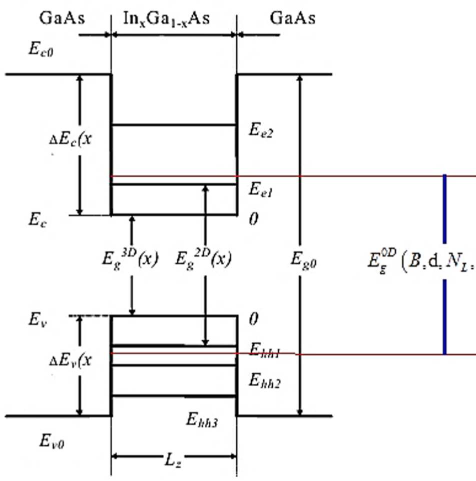


**Fig. 1.** The effect of transverse quantizing magnetic field on energy spectrum of quantum-dimensional heterostructures at low constant temperatures [1,2].

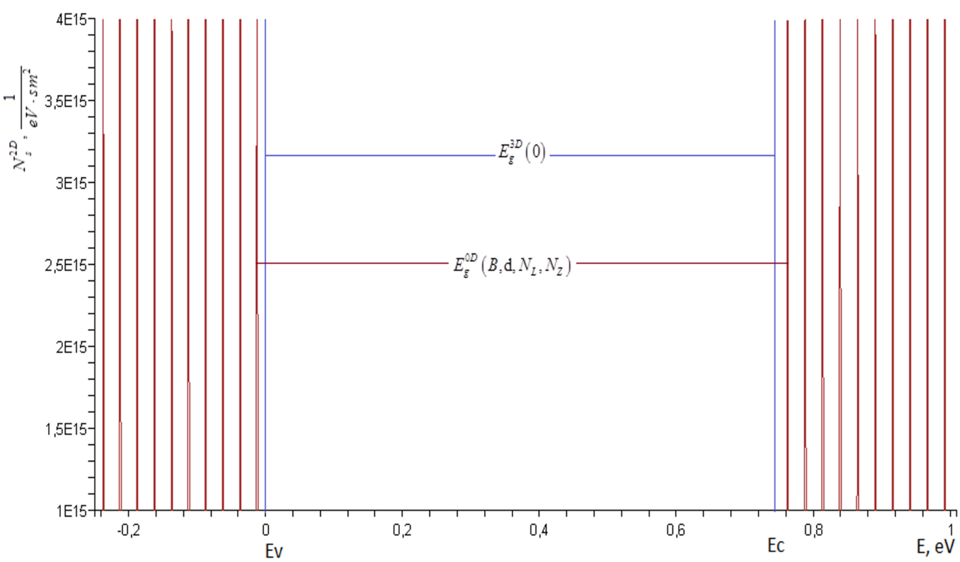


**Fig. 2.** Oscillations of density of energy states in allowed band of the $In_xGa_{1-x}As$ quantum well at T=5 K, B=10 T, and d=6 nm. Eg0 =0.75 eV.

Figure 3 shows the graphs of oscillations of the density of energy states for four different temperatures at $B$ = 10 T and $d$ = 6 nm. As can be seen, at a temperature of $T$ = 5 K, the graph of oscillations of the density of energy states has a clear boundary and a band gap $E_g^{0d}(0)=0,78\,eV$. As the temperature rises, the oscillations of the density of states change. The edges of the conduction and valence bands of the quantum well are smeared out, and the heights of discrete Landau levels of charge carriers decrease. At sufficiently high temperatures, one can observe the tail of the oscillation of the density of states in the band gap of the quantum well of the $In_xGa_{1-x}As$ solid solution. Thus, due to the thermal smearing of the Landau levels of electrons and holes, the edges of the conduction band and the valence band of the quantum well are shifted into the depth of the band gap with increasing temperature, and the band gap decreases. The dependence of the band gap of quantum wells on external factors $E_g^{2d}(B,T,d)$, is determined according to the mathematical model. The effect of magnetic field and temperature on the density of energy states of the allowed zone of the quantum well $N_s^{2d}(B,T,d)$, is calculated according to the proposed mathematical model. It follows from this that $E_g^{2d}(B,T,d)$ can be obtained from $N_s^{2d}(B,T,d)$. In this model, the concept of "mobility edges" was introduced, which manifests itself in the allowed zones of the quantum well under external influences.

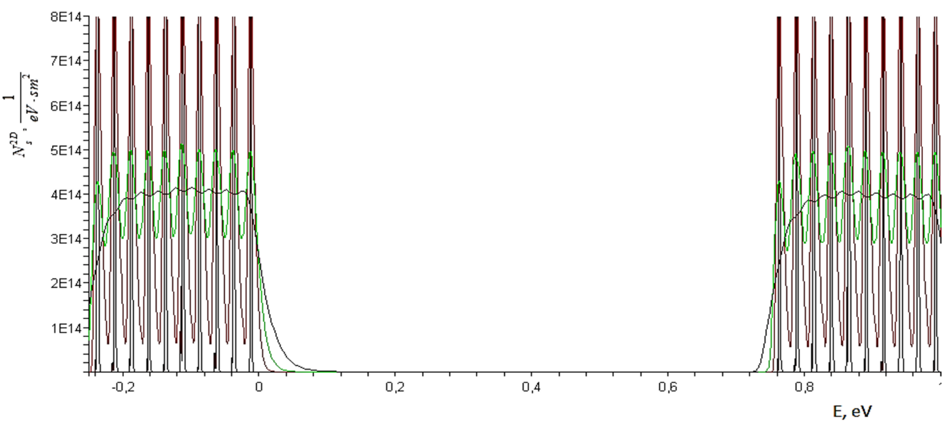


**Fig. 3.** Influence of temperature on the oscillations of the density of energy states in the allowed band of the $In_xGa_{1-x}As$ quantum well.

The effect of a transverse quantizing magnetic field on the dependence of the band gap of the $In_xGa_{1-x}As$ solid solution on the quantum well thickness. Here, the transverse quantizing magnetic fields varied from 2 T to 5 T, and the temperature was equal to $T$ = 4 K. It can be seen from these figures that when the width of the quantum well is up to 15 nm, the value of the forbidden zone changes sharply. These results were obtained using formula (8).

## 4 Conclusion

Based on the study, the following conclusions can be drawn: The effect of temperature on oscillations of the density of states in the conduction and valence bands of a quantum well under the action of a transverse quantizing magnetic field is considered. The results of calculations of the change in the band gap of a quantum well in a transverse quantizing magnetic field coincide in order of magnitude with the experimental data. Therefore, it can be concluded that thermal smearing of discrete Landau levels of charge carriers at the edges of the allowed zone of the quantum well can significantly change the band gap of nanoscale materials. The band gap's dependence on temperature and the transverse quantizing magnetic field in quantum-well heterostructural materials can be explained by the above mathematical model when the oscillations of the density of states are expanded using formulas (4) and (5). A method is developed for determining the effect of a transverse quantizing magnetic field on the temperature dependence of the band gap of a quantum well with a parabolic dispersion law. The experimental results for heterostructure with quantum-well materials are investigated using the proposed technique.

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