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Characteristics of quantum beats in InGaN/GaN quantum well

FEI GAO, GUIGUANG XIONG*

Department of Physics, Wuhan University, Wuhan 430072, China

*Corresponding author: Guiguang Xiong, ggxiong@whu.edu.cn

A *Λ*-type three level atom in the InGaN/GaN quantum wells is formed by the lowest energy level of conductive electrons and the highest sub-bands of light and heavy hole. With the excitation of the coherent light field, a quantum beat spectrum is obtained. The quantum beat spectrum can be calculated by using the theory of effective mass. Quantum beats do not exist in all polarization directions. The influence of quantum well width and the concentration of In on the spectra of quantum beats is also discussed.

Keywords: InGaN/GaN, quantum wells, quantum beats, effective mass.

1. Introduction

Semiconductor quantum structures have been attracting great interest because of their flexibility in tailoring electrical and optical properties. Besides, it becomes important to acquire better knowledge about the electrical structures, transportation properties, optical properties and the luminescence mechanism of semiconductor quantum structures, research on novel quantum structures (such as quantum dots, wires and wells) that exploit coupling and localization effects. As regards InGaN/GaN quantum wells intense interest has been aroused in materials characterized by a wide band gap, high heat conductivity, high electron saturated drift velocity and low dielectric constant [1–4]. In quantum wells, the electrons, holes and excitons have discrete energy levels because of the confinement of their motion in direction vertical to the layers of quantum wells. This makes these materials have unique physical properties useful in electronic structures and transportation, as well as unique optical properties. Observation of quantum beat is known to be an efficient method for studying a fine structure and dynamics of carrier in quantum structures. Though a lot of studies of quantum beat in quantum structure have been reported [5–8], there is no research concerning the calculation of quantum beat in InGaN/GaN quantum wells. In this paper, we have performed numerical simulations to study the quantum beat effect of the *Λ*-type three level atom system in InGaN/GaN quantum wells which is formed by the energy levels of conductive electrons and the light and heavy holes. The quantum beat spectra in InGaN/GaN quantum wells are calculated for the different well widths and constituents in different polarization directions.

2. Theory and calculation

In InGaN/GaN quantum wells growing in z direction, the band structures and the wave functions of valence band and conduction band can be described by the theory of effective mass [9, 10]. Taking account of the perturbation potential of quantum wells in the Schrödinger equation gives

$$\left[H_0 + V(\mathbf{r})\right]\Psi(\mathbf{r}) = E\,\Psi(\mathbf{r}). \tag{1}$$

The wave function can be written as a product of the envelope function $F_n(\mathbf{r})$ and the band-edge wave function $U_n(\mathbf{r})$:

$$\Psi(\mathbf{r}) = \sum_n U_n(\mathbf{r})F_n(\mathbf{r}). \tag{2}$$

For the electrons in conduction bands, $U_i(\mathbf{r}) = |C\rangle$, with $|C\rangle$ being the ground state wave function of electrons. Setting the energy level at the top of valence band to zero, the wave function and the energy level near Γ point for the electrons at the bottom of the conduction bands are:

$$F_n(k_x, k_y, z) = \frac{1}{\sqrt{L_x L_y}} \exp\left[i(k_x x + k_y y)\right] + \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi z}{L}\right), \tag{3}$$

$$E = E_g + \frac{\hbar^2\left(k_x^2 + k_y^2\right)}{2m_e^*} + \frac{\hbar^2 n^2 \pi^2}{2m_e^* L^2}. \tag{4}$$

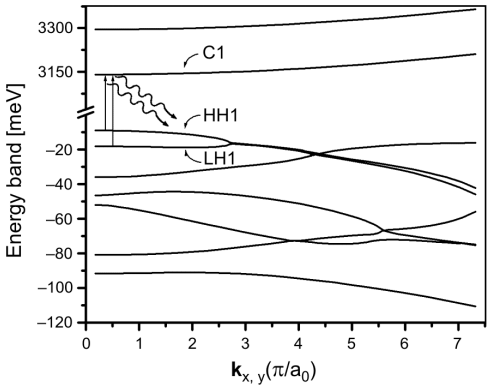

Fig. 1. Energy band as a function of **k** vertical to the z-axis in $In_{0.05}Ga_{0.95}N$ quantum wells, setting the width of the wells to 7.0 nm and the concentration of In to 0.05.

In the case of valence bands, $U_n(\mathbf{r})$ corresponds to six band-edge wave functions of holes in valence bands [10]

$$
\begin{aligned}
|v_1\rangle &= |v_{\mathrm{HH}\uparrow}\rangle = |3/2, 3/2\rangle = \frac{1}{\sqrt{2}}|(x+iy)\uparrow\rangle,\\
|v_2\rangle &= |v_{\mathrm{LH}\uparrow}\rangle = |3/2, 1/2\rangle = \frac{i}{\sqrt{6}}|(x+iy)\downarrow\rangle - i\sqrt{\frac{2}{3}}|z\uparrow\rangle,\\
|v_3\rangle &= |v_{\mathrm{SO}\uparrow}\rangle = |1/2, 1/2\rangle = \frac{1}{\sqrt{3}}|(x+iy)\downarrow\rangle + \frac{1}{\sqrt{3}}|z\uparrow\rangle,\\
|v_4\rangle &= |v_{\mathrm{SO}\downarrow}\rangle = |1/2, -1/2\rangle = -\frac{i}{\sqrt{3}}|(x-iy)\uparrow\rangle + \frac{i}{\sqrt{3}}|z\downarrow\rangle,\\
|v_5\rangle &= |v_{\mathrm{LH}\downarrow}\rangle = |3/2, -1/2\rangle = \frac{1}{\sqrt{6}}|(x-iy)\uparrow\rangle + \sqrt{\frac{2}{3}}|z\downarrow\rangle,\\
|v_6\rangle &= |v_{\mathrm{HH}\downarrow}\rangle = |3/2, -3/2\rangle = \frac{i}{\sqrt{2}}|(x+iy)\downarrow\rangle.
\end{aligned}
\tag{5}
$$

The terms of heavy holes (HH), light holes (LH) and spin-orbit split-off (SO) with different spins are included. Near the top of valence band, solving the effective mass equation, the energy levels and the wave functions of the electrons and holes can be obtained as (setting $k_z = -i(\partial/\partial z)$):

$$[H][C^m]_n = E_n[C^m]_n, \tag{6}$$

$$F_m(k_x, k_y, z) = \frac{1}{\sqrt{L_x L_y}} \exp\left[i(k_x x + k_y y)\right] + \sqrt{\frac{2}{L}} \sum_{n=1}^{N} c_n^m \sin\left(\frac{n\pi z}{L}\right). \tag{7}$$

Here $[C^m] = (C_{\mathrm{HH}\uparrow}, C_{\mathrm{LH}\uparrow}, C_{\mathrm{SO}\uparrow}, C_{\mathrm{SO}\downarrow}, C_{\mathrm{LH}\downarrow}, C_{\mathrm{HH}\downarrow})^T$ and $C^i = (C_1^i, C_2^i, \ldots, C_N^i)^T$. These are the coefficients which can be obtained by expanding the envelope function of holes. The Hamiltonian of holes is rewritten in a $6N \times 6N$ matrix form. The energy band in $In_{0.05}Ga_{0.95}N$ quantum wells is shown in Fig. 1. The details of calculation and the parameters we used can be found in our previous paper [11].

According to the transition selection rules between valence and conductive bands, the inter-band transition can exist only when $\Delta n = 0$. At room temperature, the electrons and holes in the quantum wells are distributed near the bottom of the conductive band and the top of the valence band, respectively. The quantum beat spectra are mainly caused by the excitation of the coherent light field in the Λ-type three level atom system

(formed by the highest sub-band of heavy hole HH1, the highest sub-band of light hole LH1 and the lowest conductive sub-band C1) as shown in Fig. 1. The wave function of this system can be written as a linear superposition of the wave function of HH1, LH1 and C1 [12]

$$\langle\psi| = \langle\psi_0| + a\langle\psi_1|\exp(-i\omega_{c,hh} - \tau_{hh}t) + b\langle\psi_2|\exp(-i\omega_{c,lh} - \tau_{lh}t). \tag{8}$$

Note that the electrons and holes have the double degeneration of inversion spin

$$\begin{aligned}\langle\psi_1| &= \sum_{\uparrow\downarrow}\langle \mathrm{HH}_1|,\\ \langle\psi_2| &= \sum_{\uparrow\downarrow}\langle \mathrm{LH}_1|,\\ \langle\psi_0| &= \sum_{\uparrow\downarrow}\langle \mathrm{C}_1|.\end{aligned} \tag{9}$$

The a and b are coefficients related to the pulse excitation; τ_{hh} and τ_{lh} are the relaxation items of the transition between electrons and the holes, respectively ($\tau_{hh} = \tau_{lh} = \tau$, in our calculation $\tau^{-1} = 10^{-12}$); $\omega_{ij} = (E_i - E_j)/\hbar$ is the energy separation between sub-bands i and j. The radiant power of the system can be written as:

$$\begin{aligned}I(t) \propto \left|\langle\psi(t)|\, e\mathbf{r}\,|\psi_0\rangle\right|^2 &= A\exp(-2\tau_{hh}t) + B\exp(-2\tau_{lh}t)\\ &\quad + C\exp\left[-(\tau_{hh} + \tau_{lh})t\right]\cos\left[(\omega_{c,lh} - \omega_{c,hh})t + \theta\right]\end{aligned} \tag{10}$$

where A, B, C have the following forms:

$$\begin{aligned}A &= a^2e^2\left|\sum_{c=\uparrow\downarrow,\,hh=\uparrow\downarrow}\langle c|\mathbf{r_p}|hh\rangle\right|^2,\\ B &= b^2e^2\left|\sum_{c=\uparrow\downarrow,\,hh=\uparrow\downarrow}\langle c|\mathbf{r_p}|lh\rangle\right|^2,\\ C &= abe^2\left|\sum_{c=\uparrow\downarrow,\,hh=\uparrow\downarrow}\langle c|\mathbf{r_p}|hh\rangle\right|\left|\sum_{c=\uparrow\downarrow,\,hh=\uparrow\downarrow}\langle c|\mathbf{r_p}|lh\rangle\right|\end{aligned} \tag{11}$$

while $r_p = r_p(x, y, z)$, θ is the difference between the arguments of $\sum_{c=\uparrow\downarrow,\,hh=\uparrow\downarrow}\langle c|\mathbf{r_p}|hh\rangle$ and $\sum_{c=\uparrow\downarrow,\,hh=\uparrow\downarrow}\langle c|\mathbf{r_p}|lh\rangle$. The matrix element of dipole transition between the first

sub-band of valence bands and the first sub-band of conduction band can be calculated from formulae (3), (5), (6) and (7):

$$
\begin{aligned}
x_{e\uparrow,v} &= \left(\frac{[C_1^1]_v}{\sqrt{2}} - \frac{i[C_1^4]_v}{\sqrt{3}} + \frac{[C_1^5]_v}{\sqrt{6}} \right) \Omega, \\
x_{e\downarrow,v} &= \left(\frac{i[C_1^2]_v}{\sqrt{6}} + \frac{[C_1^3]_v}{\sqrt{3}} + \frac{i[C_1^6]_v}{\sqrt{2}} \right) \Omega, \\
y_{e\uparrow,v} &= \left(\frac{i[C_1^1]_v}{\sqrt{2}} - \frac{[C_1^4]_v}{\sqrt{3}} - \frac{i[C_1^5]_v}{\sqrt{6}} \right) \Omega, \\
y_{e\downarrow,v} &= \left(\frac{[C_1^2]_v}{\sqrt{6}} + \frac{i[C_1^3]_v}{\sqrt{3}} + \frac{[C_1^6]_v}{\sqrt{2}} \right) \Omega, \\
z_{e\uparrow,v} &= \left(-i\sqrt{\frac{2}{3}}\,[C_1^2]_v + \frac{[C_1^3]_v}{\sqrt{3}} \right) \Omega, \\
z_{e\downarrow,v} &= \left(\frac{i[C_1^4]_v}{\sqrt{3}} + \sqrt{\frac{2}{3}}\,[C_1^5]_v \right) \Omega
\end{aligned}
\tag{12}
$$

where $\Omega = \dfrac{\hbar}{E_c - E_v} \sqrt{\dfrac{E_g(E_g + \Delta)}{2m_e^*\left(E_g + \dfrac{2}{3}\Delta\right)}}$ [13].

The transition from sub-band HH1 to sub-band C1 is related to $v = 1$, and the transition from sub-band LH1 to sub-band C1 is related to $v = 2$ (see Fig. 1).

3. Results and discussion

In quantum wells, the hole motion in x, y, z directions is coupled with each other. When $k_{x,y} \neq 0$, the expansion coefficients $[C_i^m]_n$ of hole wave function are not equal to zero, which means that all sub-bands of hole consist of the elements of heave, light and spin-orbit split-off hole. When $k_{x,y} = 0$, most of the coefficients $[C_i^m]_n$ return to zero, the sub-bands of hole consist of the same kind of hole-elements. Each sub-band in valence band can be labeled in this way. Though the spin-orbit split-off bands are not directly involved in the calculation of quantum beat, the spin-orbit split-off holes affect

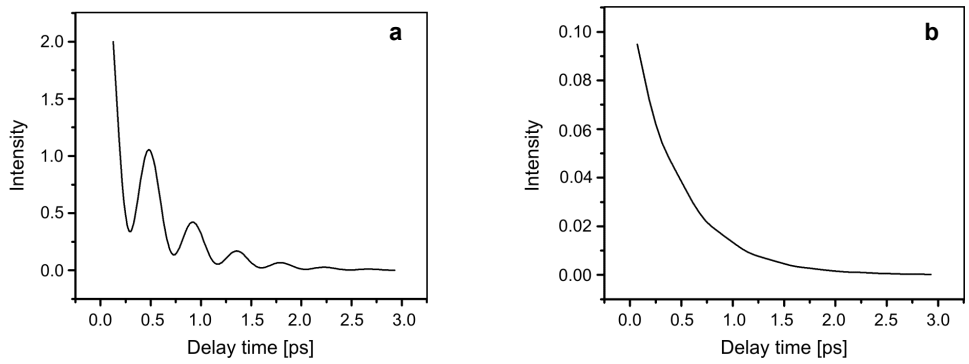

Fig. 2. Intensity of quantum beat in the directions vertical to z-axis (**a**), and parallel to z-axis (**b**).

quantum beat due to the coupling. The elements with $v = 3, 4$ in formula (12) represent the contribution of spin-orbit split-off hole to transition matrix elements between C1 and HH1, LH1.

Two spectra can be obtained from formulae (10)–(12), with the polarization direction being in parallel and vertical to z-axis, as shown in Fig. 2. The width of the well is 7 nm, the content of In is 0.05. The oscillation of intensity is obviously in x, y direction, demonstrating the quantum beat clearly. In z-direction, the spectrum of intensity is quite smooth, It can be concluded that quantum beat does not exist. Comparing the spectra in two directions, we find that the radiation intensity in x, y directions is by far bigger than that of z-direction in the course of relaxation. If we change the direction of polarization, the element of quantum beat $\exp[-(\tau_{hh} + \tau_{lh})t]\cos[(\omega_{c,\,lh} - \omega_{c,\,hh})t + \theta]$ will not change, only the transition element relating to the polarization direction will change. Thus, unless there is no the transition from HH1 or LH1 to conduction band, the quantum beats will disappear. In formula (12) there is no transition matrix element $[C_i^1]_v$ nor $[C_i^6]_v$, which shows that only the transition from LH to condcution band will take place if the polarization of incidence is towards z-direction, and only when the polarization of incidence is towards x, y direction, the transtion from HH and LH will take place together.

Two groups of quantum beat spectra in the direction vertical to z-axis are obtained by changing the width of the well and the concentration of In to understand the correlations between quantum beat and the structure and the constituents of quantum wells. When the concentration of In is set to 0.05 and the width of the wells is varied from 5 to 9 nm, a set of quantum beat spectra with different well-width are obtained, as shown in Fig. 3. Then, the width of the wells is set to 7 nm, varying the concentration of In from 0.040 to 0.060, and so, another set of quantum beat spectra with different concentration of In are obtained, as shown in Fig. 4.

It can be noted from Fig. 3 that if the concentration of In is not changed, the period of the quantum beat decreases when the width of the well decreases. This indicates

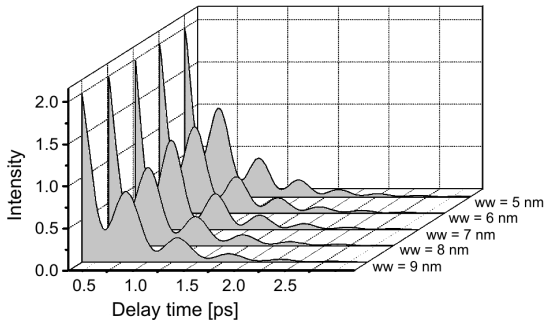

Fig. 3. Intensity *vs*. time for InGaN/GaN when the content of In is 0.05 and the width of well is changed from 5.0 to 9.0 nm.

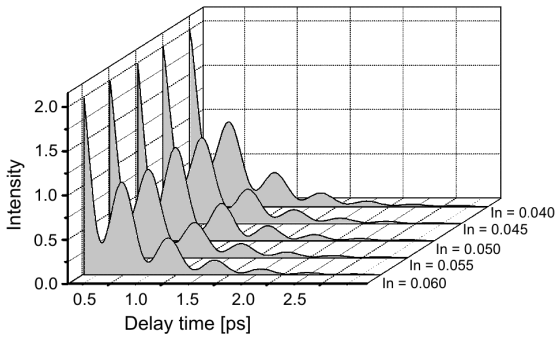

Fig. 4. Intensity *vs*. time for InGaN/GaN when the width of well is 7.0 nm and the content of In is changed from 0.040 to 0.060.

that interval between the sub-bands in valence band increases with a decrease of the well width. The oscillation amplitude increases indicate the enhancement of transition when the width of the well decreases. It can be noted from Fig. 4 that if the width of the well is given as 7.0 nm, the spectrum of quantum beat almost does not change when when concentration of In is changed from 0.040 to 0.060. This means that the change of In concentration nearby 0.050 has no influence on energy difference in sub-bands of hole and the transition between the bottom of conduction band and the top of valence band.

In conclusion, a Λ-type three level atom system is formed by the first sub-band of heavy hole, the first sub-band of light hole and the first conductive sub-band. With the excitation of the coherent light field, the quantum beat spectrum is obtained. The energy structure of quantum wells and the elements of transition matrix are calculated by using the theory of effective mass. The beats cannot exist in the direction parallel to *z*-axis because there is no transition between HH1 and C1 in *z*-direction.

The influence of quantum well width and the concentration of In on the spectrum of quantum beat is also discussed.

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