Study on electron and hole states in tilted quantum well structures

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Abstract. In this study, the energy states of electron and hole in Ga$_x$In$_{1-x}$N$_y$As$_{1-y}$/GaAs tilted quantum well structure have been theoretically investigated. The content of x and y are 0.65 and 0.005 respectively. The energy states and wave functions have been calculated by solving the Schrödinger equation in real space. The well width of 2-10 nm, barrier width of 2-10 nm and tilted layer width of 1-3 nm are considered in this work. The results show that the electron and hole energies decrease with increasing the well width and tilted layer width. The wave functions are both symmetric (ground state) and anti-symmetric (the first excited state), and spread out as the well width increases. In addition, the barrier width of couple tilted quantum well structure has also been studied. It is found that the probability of finding electron and hole are equal in both wells and the wave function within barrier layer decreases with increasing the barrier width as well. The ground state energy increases and the first excited state energy decreases as the barrier increases. As a result, the two states tend to the same level when the barrier is more than 8 nm. This is because the wide barrier can decrease the interaction between two quantum wells and makes each quantum well acts as an isolated quantum well with no interaction between them.

1. Introduction

In past decades, the semiconductor quantum well (QW) have been experimentally and theoretically studied due to their potential applications in optoelectronic devices [1-3]. A typical structure is a single QW (SQW) consisting of one well layer sandwiched between two barrier layers. The electron and hole are confined in QW layer and can create an electron-hole pair called a direct exciton. However, the direct exciton has very short lifetime. Therefore, the couple QWs (CQWs) – two wells separated by a thin barrier – have been attracted much attention since the indirect exciton with long lifetime can be created in such a structure [4]. To study the optical property, the exciton energy, binding energy and oscillator strength have been investigated for different parameter [5-8]. In addition, there are a number of research works concentrate on the electron and hole states only (not the exciton state). However, it is also very important since these states are used to calculate the exciton state and properties in the next step. The effects of structural parameters including well width, barrier width or potential profile on the single-particle energies and wave functions have been theoretically investigated [9-10].

In this work, the GaInNAs/GaAs tilted quantum well (TQW) structures are considered in order to study the effect of tilted layer on the electron and hole energies. The energy levels and wave function in single and coupled TQWs are calculated for different parameters.
2. Theoretical model

Let us consider symmetric single tilted quantum well (STQW) and coupled tilted quantum well (CTQW) consisting of a well layer sandwiched between two tilted layers as shown in figure 1.

![Schematic structures for (a) STQW and (b) CTQW.](image)

Figure 1. Schematic structures for (a) STQW and (b) CTQW.

Under the effective mass approximation, the electron and hole eigen energies are calculated by solving the Schrodinger equation which has a form:

\[
\left( -\frac{\hbar^2}{2} \frac{\partial^2}{\partial z^2} + \frac{1}{m_{e(h)} z} \frac{\partial}{\partial z} + V_{e(h)}(z) \right) \psi_{e(h)} = E_{e(h)} \psi_{e(h)},
\]

(1)

where \( E_{e(h)} \) is the electron (hole) energy, \( z \) is the electron/hole coordinate in the growth direction, \( m_{e(h)} \) is the electron (hole) effective mass, \( \psi_{e(h)} \) is the electron (hole) wave function and \( V_{e(h)}(z) \) is the electron (hole) confinement potential. The barrier layers have a potential of \( V_0 \), while the potential of tilted layers can be determined by a linear interpolation. For example, the potential of tilted layer in STQW structure is given by

\[
V(z) = -\frac{V_0}{L} \left( z \pm \frac{L_w}{2} \right).
\]

(2)

By substituting the tilted potential equation (2) into equation (1), in tilted layer is rewritten as

\[
\frac{\partial^2 \psi(\xi)}{\partial \xi^2} - \xi \psi(\xi) = 0
\]

(3)

with

\[
\xi = \left( \frac{2mV}{\hbar^2 L_r} \right)^{1/3} \left[ -z - \frac{L_w}{2} - \frac{EL_r}{V} \right].
\]

(4)

The solution of equation (3) is the combination of Airy functions \( Ai(\xi) \) and \( Bi(\xi) \), so that the wave function in tilted layer has a form [11]:

\[
\psi(\xi) = aAi(\xi) + bBi(\xi),
\]

(5)

where \( a \) and \( b \) are arbitrary constants.
3. Results and discussion

3.1. Single tilted quantum well structure (STQW)

The electron and hole energies in STQW structure have been calculated for different structural parameters. The well width of 2-10 nm and tilted width of 1-3 nm are considered. The parameters used in this calculation are given in reference [12].

![Figure 2](https://example.com/figure2.png)

Figure 2. Electron and hole energies in STQW: (a)-(b) for the ground state (e1, h1) and (c)-(d) for the first excited state (e2, h2). The wave functions are shown in (e) for electron (f) for hole.

The results are shown in figure 2. The electron and hole energies decrease with increasing the well width. It decreases rapidly for narrow well but slightly changes for wider well. The energy level decreases as the tilted width increases as well. Again, there has been found a dramatic change in energy for small tilted width. The electron ground state energy, for example, decreases from around 260 meV to 185 meV when the tilted layer of 1 nm is inserted to the structure. However, it drops only 20 meV (from 150 meV to 130 meV) when the tilted width is increased from 2 nm to 3 nm. In addition, it is found that the hole level is lower than electron level due to a lower hole potential (V0) and a higher hole mass. The wave functions are also calculated in this work. The results show that the wave functions are symmetric (ground state: e1, h1) and anti-symmetric (the first excited state: e2, h2) as can be seen in figures 2 (e)-(f). The probability of finding electron (hole) in the surrounded barrier is higher in the case of e2(h2) state compared to e1(h1) state.

3.2. Coupled tilted quantum well structure (CTQW)

We consider electron and hole energies level in CTQW structure. The tilted width id fixed to 1 nm and the well is width 4 nm. The barrier width is varied from 2 nm to 10 nm in order to study the effect of barrier width on the energy levels. The first four states of electron and hole as a function of barrier width are demonstrated in figure 3. As we expected, the electron and hole energies decreases when the tilted width is added to the structure. The ground energy (e1, h1) increases with increasing the barrier width, while the first excited state energy (e2, h2) decrease as the barrier width rises. This gives rise to energy splitting between e1-e2 (h1-h2) states. The splitting becomes smaller for wider barrier. At the barrier width of approximately 6 nm, the e1(h1) and e2(h2) levels tend to the same level which is the ground state level in STQW structure. This means that the two SQW act as an isolated single QW with no interaction between them. The same situation also happens in the case of e3-e4 (h3-h4) energy levels shown in figures 3 (c)-(d). The corresponding wave functions are demonstrated in figures 3(e)-(f). The singlet state in STQW becomes the doublet states with symmetric (e1, e3, h1, h3) and anti-symmetric (e2, e4, h2, h4) wave functions.
4. Conclusion
In this study, the single particle states in GaInNyAs/GaAs tilted quantum well structure have been theoretically investigated by solving the Schrödinger equation in real space. It is shown that the electron and hole energies decrease with increasing the well width and tilted layer width. The wave functions are both symmetric for e1(h1) and anti-symmetric for e2(h2). The wave functions are spread out when the well width is increased. For CTQW structure, the single state is split into the doublet states. The e1(h1) energy increases but the e2(h2) energy decreases, resulting the e1-e2 (h1-h2) energy splitting. This splitting becomes smaller when the barrier increases. The energies tend to the energy level of single tilted quantum well structure (STQW); e1(h1) and e2(h2) state tend to the ground state in STQW, while e3(h3) and e4(h4) states become the first excited state in STQW. As a result, each QW acts as an isolated QW. The probability of finding electron and hole are equal in both wells.

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