Effect of quantum well width on the electron and hole states in different single quantum well structures

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Abstract. In this study the electron and hole states in Al$_{0.33}$Ga$_{0.67}$As/GaAs single quantum well structures including squared QW, step QW and tilted QW, have been theoretically studied by solving the Schrodinger equation in real space. The energies and wave functions of electron and hole are calculated for different well widths. It is found that energy level of electron and hole decreases with increasing the well width. Adding step or tilted layers gives rise to the decrease of electron and hole energy levels. The ground state energy level in a tilted single quantum well structure is lower than that in a step single quantum well structure. It is also found that the energy of electron and hole ground states do not change as the width of step layer increase. This is because the ground state occupies in a lower well only. The wave functions are symmetric (ground state) and antisymmetric (the first excited state). The maximum of ground state wave function is at the central of the well and the probability of finding electron and hole in excited states are different in each region. The hole levels are lower than the electron levels due to the lower well depth and higher mass of hole compared to electron.

1. Introduction
In the past decades, the electronic and optical properties of exciton in semiconductor quantum well (QW) structure have been widely investigated because of their potential applications in optoelectronic devices. The quantum well solar cell is one of the applications which is studied in order to design the optimized solar cell with high efficiency [1-2]. The effect of structural parameters including well width, barrier width on exciton state has been theoretically studied [3-5]. The shape of potential profile is also important. Not only a squared QW but also a parabolic or triangle QW is considered [6-7]. In addition, the external field (magnetic and electric fields) has a strong effect on electron and hole states in QW [8-11].

An exciton is an electron-hole pair which is attracted to each other via the Coulomb interaction. Therefore, the electron and hole energies and wave functions in QW structure are basic quantities which is used to calculate exciton states and their properties. Here, we concentrate on the effect of potential shape on the electron and hole states. The squared, step-like and tilted QWs are studied for different parameters.
2. Method

Let us consider single quantum well structures with different potential profiles including squared QW (SQW), step-like QW (Step-QW) and tilted QW (TQW) structures. The schematic structures are shown in figure 1.

![Figure 1. Schematic structures for (a) SQW (b) Step-QW (c) TQW.](image)

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

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

(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 \( V_{e(h)} \) is the electron (hole) confinement potential. The potential of step layer and surrounded barrier layer are \( V_i \) and \( V \) respectively. For SQW and Step-QW structures, the wave function in each region is given by

\[
\psi_{e(h)} = Ae^{ikz} + Be^{-ikz},
\]

(2)

where \( A \) and \( B \) are arbitrary constants.

For TQW structure, the potential of tilted layer is obtained by a linear interpolation and has a form

\[
V(z) = \frac{-V_{el}}{L_t} \left( z \pm \frac{L_w}{2} \right)
\]

(3)

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

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

(4)

with

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

(5)

The solution of equation (1) is the combination of Airy functions \( Ai(\xi) \) and \( Bi(\xi) \), so that the wave function in tilted layer has a form [11]:

\[
\psi(\xi) = CAi(\xi) + DBi(\xi)
\]

(6)

where \( C \) and \( D \) are arbitrary constants.
3. Results and discussion

We consider the GaAs/Al\(_x\)Ga\(_{1-x}\)As QW structure with the content of x=0.33, GaAs are a well layer and AlGaAs are a barrier layer. The parameters used in the calculation are obtained from [11]. The potential \( V_1 \) is set to be \( V/2 \). The squared (\( V_1=V/2 \)), step and tilted quantum wells are considered in order to investigated the effect of potential profiles on the single-particle states. The structural parameters including well width (\( L_w=2-12 \) nm) and step-layer/tilted layer width (\( L_t=2-12 \) nm) are studied. The results show that the electron and hole energies in all structures decreases with increasing the well width. Figure 2 and figure 3 show the ground state and the first excited state for \( L_w=2, 6, 10 \) nm compared to the energies in SQW structure (symbol).

![Figure 2](image2.png)

**Figure 2.** Electron and hole energies in Step-QW structure: (a),(c) for the ground state (GS) and (b),(d) for the first excited state (1\(^{st}\)ES). The wave functions are shown in (e) for electron (f) for hole.

![Figure 3](image3.png)

**Figure 3.** Electron and hole energies in TQW structure: (a) and (c) for the ground state (GS) and (b) and (d) for the first excited state (1\(^{st}\)ES). The wave functions are shown in (e) for electron (f) for hole.
For Step-QW, there is no difference in the ground state energies (both electron and hole cases) when the step-layer width is changed. This is because the ground state electron and hole are confined in a lower well (see the wave function in figure 2(e) and (f), so that the change of step-layer width does not cause the change of ground state energy. For the first excited state the step-layer width plays an important role since the state is localized in the step layer. Noted that its energy is larger than the potential $V_1$ ($V_1 = 133.74$ meV for electron and $V_1 = 72.015$ meV for hole). However, the energies for all values of $L_t$ tend to the same level at wider well width. It happens earlier in the case of hole due to a heavier hole mass and a lower hole potential.

For TQW structure, the pictures of the ground state and the first excited state energies look similar. The electron and hole energies decrease as the tilted width increases, but a small change in energy can be observed when the tilted layer is increased from 6 nm to 10 nm. The corresponding wave functions are demonstrated in figure 3(e) and (f). It is found that the wave functions are symmetric ($e_1 e_3 h_1 h_3$) and antisymmetric ($e_2 e_4 h_2 h_4$).

4. Conclusions
In this work, we calculate the electron and hole energy levels and their wave in Al$_{0.33}$Ga$_{0.67}$As/GaAs single quantum well structures including squared QW, step QW and tilted QW by solving the Schrodinger equation in real space. It is found that the energies of electron and hole decrease when the quantum well width and the step/tilted layer width are increased. The energy levels in the tilted QW structure smoothly change with tilted width because the potential in tilted layer is smoothly changed from the surrounded barrier potential $V$ to the well potential. The situation is different in the case of step QW. The ground state energies of electron and hole do not change when the width of the step layer is increased. This is due to the ground state occupies in the lower well only. Therefore, the tilted layer does not affect to its energy level. The state strongly depends on the well width. The wave functions of electron and hole is both symmetric ($e_1 e_3 h_1 h_3$) and antisymmetric ($e_2 e_4 h_2 h_4$). The highest probability of finding electron (hole) is at the center of the well. In addition, it is found that the energy levels of hole is lower than the electron energy levels because of the larger hole mass and lower hole potential depth.

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