Intersubband electron transition across a staircase potential containing quantum wells: light emission

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Abstract

We present a theoretical investigation of a novel staircase-like light emitter based on the GaAs/Ga\textsubscript{1−x}Al\textsubscript{x}As material system. The emission wavelength is around 12 µm. The device operation is based on the intersubband bound-to-bound transition. The energy band profile of the structure has been solved self-consistently. We have also calculated the oscillator strength.

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1. Introduction

In 1970 Kasarinov and Suris proposed that light amplification could be achieved by photon-assisted tunneling at photon energies equal to the energy difference between the ground state and adjacent excited states of quantum wells [1]. Following this proposal, the first quantum cascade laser (QCL), in which optical transitions occur in the multiple active regions separated by injectors, was introduced in 1994 [2]. Since then there has been a growing interest in QCL structures because of their operation range spanning...
Fig. 1. Conduction band profile of staircase structure with quantum wells at the flat band condition. The Fermi level is shown with dashed lines. The quasi-barrier on the left-hand side is shown with a bold dotted line.

Fig. 2. Sample structure with quantum wells and barriers where the concentration $x$ varies from 0 to 0.45. The exact

from mid-to-far infrared wavelengths between 3, 5 and 24 µm. Furthermore, high peak power levels make them desirable for applications [3], such as ultrahigh resolution spectroscopy, ultrahigh sensitivity gas sensing systems and military technologies. A large number of QCL structures to date have been investigated. These include applications as distributed feedback (DFB) lasers [4], GaInAs/AlInAs based superlattice (SL) lasers [5], chirped SL lasers [6], GaAs/AlGaAs based QCL [7] and InAs/GaSb/AlSb type-II cascade structures [8].

In our work, we present the theoretical study of a novel staircase structure, which is based on a GaAs/AlGaAs material system and can be operated between 8 µm and 12 µm ranges by changing the barrier height and well width. The structure design has been inspired from QCLs. The difference between them is that the potential energy of the quantum wells and barriers changes with varying Al concentration. The potential profile of the structure is given schematically in Fig. 1. The sample will be doped as the Fermi energy level to be placed below the ground state of the first quantum well and continue throughout the sample as shown in Fig. 1, and also the Fermi level of the system must be chosen such that

$$|\epsilon_{\text{GaAs}} - \epsilon_f| + |\epsilon_{\text{AlGaAs}} - \epsilon_f| \cong \Delta \epsilon_c$$

where $\Delta \epsilon_c$ is the conduction band discontinuity of AlGaAs–GaAs; then we will be able to prevent band bending at wells/barriers interfaces. The structure has been designed, as the excited energy states of the quantum wells are 25 meV lower than the barrier heights at room temperature, as shown in Fig. 2. Therefore the electron wave functions at the excited states are localized in quantum wells.

2. Device structure

The device structure, which we investigate, is an $n^+-i-n$ three well system containing quantum wells and barriers where the concentration $x$ varies from 0 to 0.45. The exact
Fig. 2. Conduction band profile and squared electron wave functions of staircase light emitter at the flat band condition.

Table 1
Calculated potentials and energies for barriers ($b$) and wells ($w$)

<table>
<thead>
<tr>
<th>$n$</th>
<th>$V_b^W (V_n^w)$ [eV]</th>
<th>$z_b^W (z_n^w)$ [Å]</th>
<th>$E_{n_{i}}^{w} - E_{n_{f}}^{w}$ [eV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.275(0.11)</td>
<td>150(186)</td>
<td>0.144–0.237</td>
</tr>
<tr>
<td>2</td>
<td>0.363(0.1837)</td>
<td>246(282)</td>
<td>0.223–0.329</td>
</tr>
<tr>
<td>3</td>
<td>0.440(0.275)</td>
<td>336(386)</td>
<td>0.307–0.399</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td>451</td>
<td></td>
</tr>
</tbody>
</table>

Table 2
Summary of device structure

<table>
<thead>
<tr>
<th>Composition (x)</th>
<th>Thickness (Å)</th>
<th>Doping (cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quasi well</td>
<td>0</td>
<td>150</td>
</tr>
<tr>
<td>First barrier</td>
<td>0.25</td>
<td>36</td>
</tr>
<tr>
<td>First well</td>
<td>0.1</td>
<td>60</td>
</tr>
<tr>
<td>Second barrier</td>
<td>0.33</td>
<td>36</td>
</tr>
<tr>
<td>Second well</td>
<td>0.167</td>
<td>54</td>
</tr>
<tr>
<td>Third barrier</td>
<td>0.4</td>
<td>50</td>
</tr>
<tr>
<td>Third well</td>
<td>0.25</td>
<td>65</td>
</tr>
<tr>
<td>Fourth barrier</td>
<td>0.45</td>
<td>169</td>
</tr>
</tbody>
</table>

Composition and thickness of all quantum wells and barriers are given in Table 2. The resulting device parameters including potentials and bound state energies are given in Table 1. $z_n^W$ ($z_n^b$) shows the distance of the left-hand side of the $n$th well (barrier) from the origin.
3. Theory

The potential energy of the system shown in Fig. 1 can be given as

\[ V = V_G + V_{\text{max}} \]  

(1)

where

\[ V_G = \sum_{n=1}^{3} V_G^n \]

\[ V_{\text{max}} = V_{\text{max}} S(z - z^b) \]

and

\[ V^n_G = \begin{cases} V^n_b, & z^n_b < z < z^n_w \\ V^n_w, & z^n_w < z < z^n_{b+1} \\ 0, & \text{elsewhere} \end{cases} \]

The Hamiltonian of the system can be written as

\[ H = \frac{p^2}{2m} + V. \]  

(2)

The eigenfunctions of the Schrödinger equation are of the form, in the wells and barriers, respectively,

\[ \psi_{\text{well}} = A_n e^{ik_w^n z} + B_n e^{-ik_w^n z} \]

\[ \psi_{\text{barrier}} = C_n e^{k_b^n z} + B_n e^{-k_b^n z}. \]  

(3)

Here the \( k_w^n \) and \( k_b^n \) are the wave numbers of wells and barriers, for the effective mass approximation and they are given as

\[ k_w^n = \sqrt{\frac{2m^*}{\hbar^2}(E - V^n_w)} \]

\[ k_b^n = \sqrt{\frac{2m^*}{\hbar^2}(V^n_b - E)} \]  

(4)

respectively.

In order to calculate the wave functions, we placed a quasi-barrier on the left-hand side of the structure with potential height, \( V_{\text{max}} \), as shown in Fig. 1 with bold dotted lines. Thus we obtain the decaying plane waves in this region. Then we perform a 12 \times 12 secular matrix, which can be solved by using \( \text{Det} [H_{12 \times 12}] = 0 \). The actual energies of the system can be separated from quasi-levels using confined wave functions. The width of the quasi-wells is chosen so that confinement energies in the wells are not affected.

We then applied an electric field in order to study the subband transitions under applied bias. The potential energy of the system can be written for the wells and barriers as

\[ V^n_{w,F} = V^n_w + eFz \]

\[ V^n_{b,F} = V^n_b + eFz \]  

(5)
where $F$ is the applied electric field. The solution of the Schrödinger equation can be written as

\[
\frac{\partial^2 \psi_n^w}{\partial \tilde{Z}_n^w} - \tilde{Z}_n^w \psi_n^w (\tilde{Z}_n^w) = 0
\]

\[
\frac{\partial^2 \psi_n^b}{\partial \tilde{Z}_n^b} - \tilde{Z}_n^b \psi_n^b (\tilde{Z}_n^b) = 0
\]

(6)

where

\[
\tilde{Z}_n^w = -\left[ \frac{\pi}{F} \right]^\frac{1}{3} \left[ (\tilde{E} - \tilde{V}_n^w) + \tilde{q} \tilde{F} \tilde{z} \right]
\]

(7)

\[
\tilde{Z}_n^b = -\left[ \frac{\pi}{F} \right]^\frac{1}{3} \left[ (\tilde{V}_n^b - \tilde{E}) + \tilde{q} \tilde{F} \tilde{z} \right]
\]

(8)

which can be calculated using the normalizations

\[
\tilde{E} = \frac{E}{E_0}, \quad \tilde{F} = \frac{qFL}{E_0}, \quad \tilde{z} = \frac{z}{L}, \quad E_0 = \frac{\pi^2 \hbar^2}{2m^*L^2}
\]

where $\tilde{q} = +1 (-1)$ represents holes (electrons) in the structure having width of $L = z_{\text{max}}$. The solutions of Eq. (6) in the well and barrier regions are given by Airy functions as

\[
\psi_n^w (\tilde{Z}_n^w) = E_n Ai (\tilde{Z}_n^w) + F_n Bi (\tilde{Z}_n^w)
\]

\[
\psi_n^b (\tilde{Z}_n^b) = G_n Ai (\tilde{Z}_n^b) + H_n Bi (\tilde{Z}_n^b)
\]

(9)

where $E_n, F_n, G_n$ and $H_n$ are coefficients which can be determined from the $12 \times 12$ secular matrix obtained by normalization conditions and the continuity of wave functions at $\tilde{z}_n^w$ and $\tilde{z}_n^b$.

We have also calculated the oscillator strength of the structure, which is given by

\[
f = \frac{2m^* (E_{f}^w - E_{i}^w)}{\hbar} - \int_0^{z_{\text{max}}} \psi_f^* z \psi_i \, dz
\]

(10)

where $E_{f}^w$ and $E_{i}^w$ are the excited state energy level and ground state energy level of the quantum wells, respectively.

4. Results and conclusion

At the flat band condition the calculated energy levels of the quantum wells and squared wave functions are shown in Table 1 and Fig. 2, respectively. The energy level differences between $E_{1,f}^w$ and $E_{1,i}^w$, $E_{2,f}^w$ and $E_{2,i}^w$, and $E_{3,f}^w$ and $E_{3,i}^w$ are also calculated from Table 1 as 14 and 22 meV, respectively. These energy differences will decrease with applied bias and still become comparable with optical phonon energy. Therefore, light emission and carrier injection due to tunneling through barriers by absorbing or emitting optical phonons can occur at room temperature. Our calculations show that the consecutive energy levels of adjacent wells coincide at an electric field of $2.1 \, \text{kV/cm}$, as shown in Fig. 3. Here electrons make a transition from the excited state to the ground state by emitting photons followed by
tunneling through the barrier into the excited state of an adjacent quantum well. The energy difference between the excited state and the ground state of the second quantum well is found to be 106 meV, which corresponds to a wavelength around 12 µm. As seen from the Table 1, the light emission photon energies vary from 92 to 106 meV.

We have solved the potential band profile of the structure self-consistently using the technique given in [9], and the profile is shown in Fig. 4. As seen from the figure, band bending has occurred due to the built-in potential which is around 0.26 V. Because of this built-in potential, the consecutive energy levels of adjacent wells coincide around an electric field of 30 kV/cm in fact.
We have also calculated the oscillator strength versus electric field, while the structure is operating as a light emitter, shown in Fig. 5. There are two important points in our structure. One is the high oscillator strength to increase the subband transition probability, and the other is the high probability for tunneling. There is no possibility of having both maximum oscillator strength and maximum tunneling, because of the localization of the wave functions in two adjacent wells while tunneling. This forces the oscillator strength to decrease due to Eq. (10). In our structure tunneling is more important than subband transition in order to ensure the system continuity. So we have preferred the electric field of 2.1 kV/cm to obtain high tunneling probability.

Emission wavelengths lower than 12 µm can be obtained by changing the composition $x$ to unity (AlAs). This composition will allow us to obtain large conduction band discontinuities. Therefore quantum wells with high potential barriers can be placed into the system.

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