EQUIDISTANT ELECTRONIC STATES IN DIFFUSED GaAs/AlGaAs QUANTUM WELLS

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Abstract. We show that by a suitable choice of annealing time and temperature it is possible to obtain an interdiffused GaAs/AlGaAs quantum well with a nearly equidistant energy spectrum, very similar to that of a parabolic QW.

1. Introduction

Quantum wells (QWs) with equidistant energy levels are important for various advanced device fabrication. Parabolic QWs have this feature but they are difficult to grow. Two approaches are mainly used, the analog alloy method and the digital alloy method [1]. The first approach is technically complicated and the second one has the limitations of the digital approximation. It has been shown recently that an interdiffused GaAs/AlGaAs QW may possess an energy spectrum very close to the energy spectrum of a parabolic well [2]. In this study we investigate the electronic states in diffused (001) GaAs/AlGaAs QWs for different QW widths and diffusion lengths. The calculations are made using the envelope-function approximation. It is shown that an equidistant energy spectrum can be obtained in diffused QWs by adjusting the diffusion length, i.e. the annealing time and/or temperature. The results can be used to obtain structures with the desired equidistant spectrum by means of annealing rectangular QWs.

2. Calculation details

The width \( L_w \) of the initial (as-grown) GaAs/Al\(_{0.2}\)Ga\(_{0.8}\)As rectangular QW has been varied from 32 to 100 monolayers (ML) with a step of 4 ML (1 ML = 0.283 nm). For thinner wells the number of electron levels is less than 3 and the question of equidistance cannot be posed. The Al concentration profile \( C(z) \) across the well after diffusion is [3]:

\[
C(z) = C_A + 0.5 \left( C_W - C_B \right) \text{erf}(h - z)/L_D + \text{erf}(h + z)/L_D \ .
\]

Here \( z \) is the distance from the well centre; \( C_W \) and \( C_B \) are the initial Al concentrations in the
well and in the barriers, respectively; \( h = L_w/2 \); \( L_D \) is the diffusion length; and \( \text{erf}(x) \) is the error function. For each value of \( L_w \) diffusion lengths from 16 to 56 ML (with a step of 2 ML) are considered.

The electronic structure at the \( \Gamma \) point of the two-dimensional Brillouin zone is calculated using the envelope function approximation [4]. The confinement energies for electrons are computed by solving numerically the Schrödinger equation applying the finite differences method. The electron effective masses (in free electron mass units) used are 0.0665 for GaAs, 0.15 for AlAs [5], and a linear interpolation for \( \text{Al}_{1-x}\text{Ga}_x\text{As} \). The bandgap of \( \text{Al}_{1-x}\text{Ga}_x\text{As} \) at the \( \Gamma \) minimum is deduced from [5]: \( E_g(x) = 1.519 + 1.087 \times 0.438 \times x^2 \). The conduction to valence band offset ratio is assumed to be 66/34 [6].

3. Equidistant energy levels

The sets of electron levels corresponding to different combinations of \( L_w \) and \( L_D \) are analysed using a parameter of equidistance and a criterion for equidistance. They are defined as follows: let \( E(n) \) be the electron level energy as a function of the level number, \( n \). For a perfectly equidistant set of levels the function \( E(n) \) is a straight line and its second derivative \( d^2E(n)/dn^2 \) is zero for each value of \( n \) (where it is defined). The parameter of equidistance, \( \Delta 2 \), for a set of \( m \) levels is defined as the normalised sum of the absolute values of the second derivatives of \( E(n) \), weighted with the corresponding energies:

\[
\Delta 2 = \frac{1}{(m-2)} \sum_{n=2}^{m-1} \frac{1}{E(n)} \left| \frac{d^2 E(n)}{dn^2} \right|
\]

(2)

![Equidistance parameter Δ2 as a function of the initial QW width, \( L_w \), and the diffusion length, \( L_D \), if 3, 4, or 5 levels are considered.](image)

Figure 1. Equidistance parameter \( \Delta 2 \) as a function of the initial QW width, \( L_w \), and the diffusion length, \( L_D \), if 3 (a), 4 (b) or 5 (c) levels are considered.

The criterion for equidistance is that looking for \( m \) equidistant levels we evaluate of \( L_w \) and \( L_D \). Fig. 1a, b and c show that the QWs which number of electron is represented by a high value (30%) of \( \Delta 2 \) nearly equidistant for QWs in the region \( \Delta 2 \) is only 0.08%. This value corresponds to 0.04 meV. When 4 or 5 levels are considered the same (Fig.1b and c), although 3% for 4 levels and 2% for 5 levels, respectively, and shifts toward QWs with the best \( \Delta 2 \) values are summarized in Table 1.

<table>
<thead>
<tr>
<th>Number of levels considered</th>
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<tbody>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td>5</td>
</tr>
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</table>

4. Diffusion time and temperature

Using the fact that \( L_D^2 = 4D \cdot t \) and \( D \) is the diffusion value of \( L_D \), recent studies [7] report with 3.6 eV. Using these values we calculated lead to three diffusion lengths: 28, 30 and 32 ML, respectively. As is by annealing at reasonable temperature.
The criterion for equidistance is therefore the minimum of this parameter. Thus, when looking for \( m \) equidistant levels we evaluate \( \Delta Z \) for each set of levels and plot it as a function of \( L_W \) and \( L_D \). Fig. 1a), b) and c) show the plots \( \Delta Z(L_W, L_D) \) for \( m = 3, 4 \) and 5, respectively. The QWs which number of electron states is less than \( m \) are not interesting and are represented by a high value (30\%) of \( \Delta Z \). It is seen from Fig.1a that the first three levels are nearly equidistant for QWs in the region around the point \((L_W = 96 \text{ ML}, L_D = 30 \text{ ML})\), where \( \Delta Z \) is only 0.08\%. This value corresponds to a deviation from the equidistance as small as 0.04 meV. When 4 or 5 levels are considered the region of nearly equidistant levels remains roughly the same (Fig.1b and c), although the minimum of \( \Delta Z \) slightly increases up to 1.37\% and 2\%, respectively, and shifts towards a neighbour point \((L_W = 100 \text{ ML}, L_D = 32 \text{ ML})\). The QWs with the best \( \Delta Z \) values are summarised in Table 1.

<table>
<thead>
<tr>
<th>Number of levels</th>
<th>( L_W ) (ML)</th>
<th>( L_D ) (ML)</th>
<th>( \Delta Z ) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>92</td>
<td>28</td>
<td>0.14</td>
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<td></td>
<td>96</td>
<td>30</td>
<td>0.08</td>
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<td></td>
<td>100</td>
<td>32</td>
<td>0.25</td>
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<td>92</td>
<td>28</td>
<td>1.62</td>
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</tr>
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<td>30</td>
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<tr>
<td></td>
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<td>32</td>
<td>2.00</td>
</tr>
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</table>

4. Diffusion time and temperature

Using the fact that \( L_D^2 = 4D \tau \) and \( D = D_0 \exp(-E_a/kT) \), where \( E_a \) is the activation energy of diffusion, one can find the diffusion time \( \tau \) and temperature \( T \) needed to obtain the desired value of \( L_D \). Recent studies [7] report for the diffusion coefficient \( D_0 = 0.2 \text{ cm}^2/\text{s} \) and \( E_a = 3.6 \text{ eV} \). Using these values we calculate and present on Fig. 2 combinations of \( \tau \) and \( T \), which lead to three diffusion lengths: 28, 30 and 32 ML. According to Table 1 these three values are the most interesting in our case. As seen from Fig.2, such diffusion lengths can be achieved by annealing at reasonable temperatures for reasonable times.
Figure 2. Diffusion time and temperature giving the desired values of $L_D$.

5. Conclusion

The electron level energies are calculated for a large number of interdiffused AlGaAs/GaAs QWs varying the QW width and diffusion length. Interdiffused QWs with nearly equidistant energy levels up to the 4th - 5th levels are found for certain values of $L_W$ and $L_D$. The time and temperature needed to obtain the desired energy spectra by thermal annealing are calculated.

Further studies will include varying the initial Al concentration in the well and the barriers, using more recent and precise data for the interdiffusion coefficient and experimental verification.

Acknowledgements

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References:


