

## ELECTRONIC STATES OF DIFFUSED GaAs/AlGaAs QUANTUM WIRES

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The electronic states and optical transition energies in diffused V-shaped GaAs/AlGaAs quantum wires (QWRs) are studied by means of the envelope-function approximation. It is demonstrated that the energy spectrum and optical properties of QWRs can be essentially modified by diffusion, the modification being larger for thinner wires. Furthermore, diffusion is simulated in real V-shaped GaAs/AlGaAs QWRs used in photoconductivity spectral measurements. From the comparison between the calculated and the experimentally obtained optical transition energies, an indication of the high interface quality of the samples is found.

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### 1. Introduction

The electronic and optical properties of compositionally graded semiconductor structures are strongly sensitive to the potential profile, and give access to a variety of new phenomena and devices [1, 2]. Subjects of special interest are graded quantum wires (QWRs), the composition of which varies with distance along the growth direction. In this study, we investigate theoretically the electronic states for different diffusion lengths in diffused V-shaped GaAs/AlGaAs QWRs grown along the (001) direction. The calculations are made within the framework of the envelope-function model, by using a simple approximation [1].

### 2. Calculation details

Two V-shaped GaAs/Al<sub>0.4</sub>Ga<sub>0.6</sub>As QWRs are considered, which have similar curvatures, but different thicknesses in the central part (Fig. 1). In the first one, which is a model structure, the central width is 16 monolayers (ML), while the lateral dimension of the crescent is about 140 MLs (1 ML = 0.283 nm). The second structure corresponds to an experimental sample [3]. Its crescent shape, taken from a cross-sectional high-resolution transmission electron microscopy image, is 31 ML (9 nm) thick in the centre and about 212 ML (60 nm) wide in the lateral direction. The shapes of the top and bottom crescents of the first QWR are chosen to be parabolas with curvatures corresponding to the shape of the second (experimental) structure.

To calculate the bound state energies a simple approach is applied, separately considering the carrier confinement in the growth direction X and the Y direction, which follows the crescent run. This is possible because the crescent width is much smaller than its length, and varies slowly along Y [1]. Then the electron and hole wavefunctions,  $\Psi$ , factorize to  $\Psi(x,y) = \chi(x) \cdot \phi(y)$ , and the two-dimensional Schrödinger equation can be approximated by two coupled one-dimensional equations for  $\chi(x)$  and  $\phi(y)$ , respectively. Thus, the crescent is considered as being formed by many quantum wells (QWs) with different thicknesses. The carrier confinement energy levels are

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calculated for each QW. The results for a given level build up the shape of the lateral confinement potential in the equation for  $\phi(y)$ . Thus, each level in the individual QWs gives rise to a series of levels, corresponding to the quasi-one dimensional confinement. A simple one-band envelope

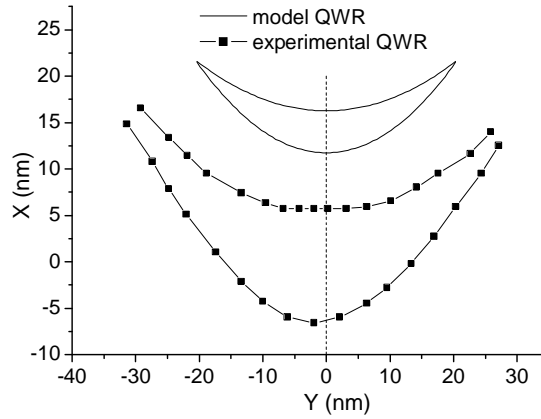


Fig. 1. QWR profiles of the samples used in the calculations.

function approximation model and the material parameters from [4] have been used in a numerical solution of the envelope function equation, by the finite-difference method. In a first approximation, a constant diffusion coefficient is used in the diffusion equation [5,6], resulting in a simple solution for the Al concentration profile  $C(z)$  across the well after diffusion [5]:

$$C(z) = C_B + \frac{C_W - C_B}{2} \left[ \operatorname{erf}\left(\frac{h-z}{L_D}\right) + \operatorname{erf}\left(\frac{h+z}{L_D}\right) \right] \quad (1)$$

Here,  $z$  is the distance from the well centre;  $C_W$  and  $C_B$  are the initial Al concentrations in the wire and in the AlGaAs barriers, respectively,  $h = L_W/2$ ,  $L_W$  is the well width before diffusion,  $L_D$  is the diffusion length, and  $\operatorname{erf}(x)$  is the error function.

### 3. Results and discussion

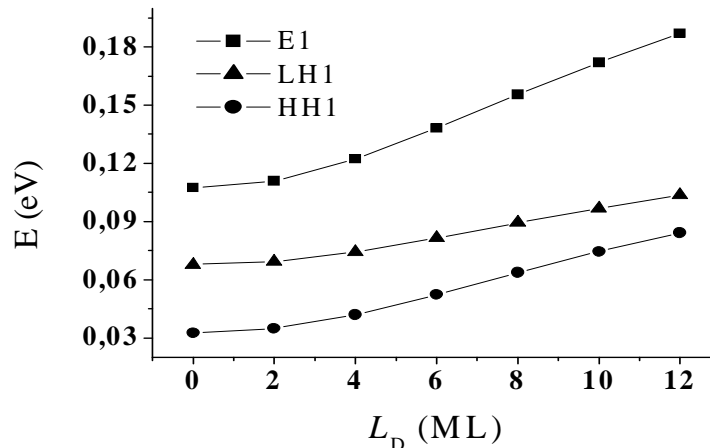


Fig. 2. Calculated energies as a function of the diffusion length for the electron, heavy hole and light hole levels in the model QWR.

The calculated energies for the lowest electron (E), heavy hole (HH) and light hole (LH) levels in the model QWR are shown in Fig. 2 as a function of the diffusion length. The energies of electrons (holes) are measured from the bulk GaAs conduction (valence) band. The modification of the bound state energies in QWs with diffusion is a well known effect [6], which has found several applications in practice. To our knowledge, this problem has not been studied in QWRs. It is reasonable to expect that for small and moderate diffusion lengths, the lowest energy levels in a QWR will increase with the increase of  $L_D$ , as happens in the case of QWs. Indeed, Fig. 2 reveals such behaviour. For  $L_D = 8$  ML, the increase in the energy with respect to the case  $L_D = 0$  is 40 meV for electrons, 30 meV for HH and 21 meV for LH, while for  $L_D = 12$  ML the corresponding values are as high as 80, 52 and 36 meV, respectively. This result shows that the energy spectrum of QWRs, and therefore their optical properties, can be strongly modified by intentionally provoked interdiffusion of material components across the interfaces.

Furthermore, we study the effect of the diffusion on the second sample. The calculated bound state energies for the first two E, HH and LH levels are shown in Fig. 3a. Again, an increase is observed, but it is less pronounced in comparison with the first QWR. The increase is only 10 to 20 meV even for the second energy levels. This is connected to the wider crescent in the present case. Indeed, solving the equation for  $\chi(x)$ , we consider the lowest electron and hole energy states, which are localised in the central part of the QWs. As the interdiffusion modifies the potential predominantly in the interface regions of the QWs, the considered energy states will be less affected by an increasing  $L_D$  in wider than in thinner wells.

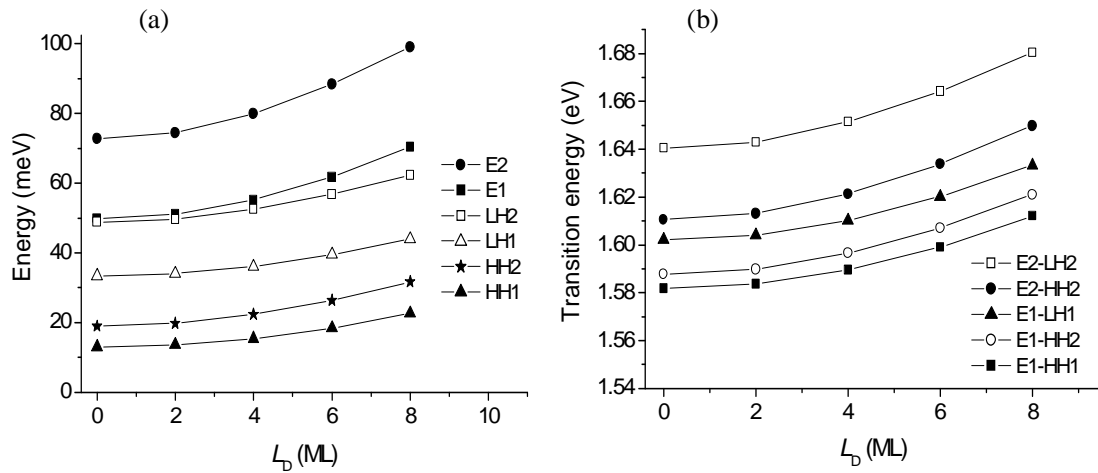


Fig. 3. Calculated energies as a function of the diffusion length in the experimental QWR sample, from [3]: a) for electrons and holes bound states; b) for the lowest optical transitions.

Table 1. Comparison between the optical transition energies (in meV) observed in the photoconductivity spectra [3] and the corresponding energies calculated for a number of diffusion lengths. For each  $L_D$ , the calculated values have been shifted to obtain coincidence with experiment for the E1-HH1 transition.

Transition	Experimental value	$L_D=0$ ML	$L_D=2$ ML	$L_D=4$ ML	$L_D=6$ ML	$L_D=8$ ML
E1-HH1	1542	1542.0	1542.0	1542.0	1542.0	1542.0
E1-HH2	1547	1548.0	1548.2	1549.0	1550.0	1551.0
E1-LH1	1553	1561.0	1562.4	1562.7	1563.1	1563.2

Fig. 3b represents the energies of some optical transitions as a function of the diffusion length, calculated from the bound state energies and using the value of the GaAs band-gap at 0K (1.519 eV). They increase with increasing  $L_D$ , in accordance with the results in Fig. 3a. In our previous paper [3], the same QWR sample has been studied by means of photoconductivity spectroscopy at a temperature of 65 K. The three lowest optical transitions, observed in the experimental spectra as peak structures, have been identified as E1-HH1, E1-HH2 and E1-LH1, respectively [3]. A comparison of the energy positions of these photoconductivity peak structures with the transition energies calculated for different diffusion lengths can give information about an eventual grading on the QWR interfaces. In order to take into account excitonic effects, as well as the temperature dependence of the GaAs band-gap, before the comparison the calculated energies are shifted downwards so that the values corresponding to the E1-HH1 transitions coincide with the experimental one. The shift is different for calculations employing different values of  $L_D$ . The calculated and experimentally obtained energies depicted above are compared in Table 1. When  $L_D$  increases, the energies for the E1-HH2 and E1-LH1 transitions shift further and further away from the experimental values. The best correspondence between theory and experiment is found for zero diffusion length, which indicates a high interface quality for the experimental sample.

#### 4. Conclusions

We have demonstrated the possibility for interdiffusion-induced modification of the QWR optical properties using V-shaped GaAs/AlGaAs QWRs. It could be expected that similar behaviour also takes place in other QWRs systems. Interdiffusion of the material components across the QWR interfaces could be intentionally realised, e.g. by sample annealing. As in the case of QWs, such an approach could lead to many useful applications in practice. Diffusion simulation in real V-shaped GaAs/AlGaAs QWRs has allowed us to obtain an indication of the good interface quality in the samples.

#### Acknowledgements

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