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# Electron states energies and wave functions of V-shaped quantum wires with graded interfaces

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We have studied the effect of graded interfaces on the bound electron states energies and wave functions of a model V-shaped GaAs/AlGaAs quantum wire (QWR). The calculations are performed by means of the envelope-function approximation combined with the so called adiabatic approximation approach for V-shaped QWRs. The interface grading is modelled by a concentration profile, obtained as a result of the material inter-diffusion across the interfaces. It is found that with increased interface grading, the energies of the QWR bound states increase monotonically, while the ground state wave function shape reveals a non-monotonic behaviour – it initially shrinks in both directions and then broadens again predominantly in the growth direction. The obtained results show that the energy levels and wave function localization in quantum wires can be modified in a controllable manner by intentionally provoked inter-diffusion of material components across the interfaces.

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## 1. Introduction

The modification of the electronic states and optical properties of quantum nanostructures by means of purposely induced interface grading has attracted a growing interest during the last decades because of various potential applications in integrated photonic circuits. The material intermixing by means of (thermally induced) inter-diffusion is a prospective technique for fine tuning the shape and size and thus the optical properties of nanostructures at a post-growth level [1-3]. The modification of the bound states and optical transition energies in quantum wells (QWs) by means of inter-diffusion is a well-known effect [1,4-6],which has found various applications [7,8]. More recent studies [2,3] report promising results on intermixing in quantum dots, such as a substantial blue shift of the optical band-gap energy and sharper photoluminescence lines.

In quantum wires (QWRs), controlled spatially resolved interface grading, e.g. by thermally induced inter-diffusion, could be used for selective modification of their properties along the wire direction, in order to obtain new integrated device structures. However, there are relatively less studies on the inter-diffusion effects in QWRs. In our previous work [9] we have modelled inter-diffused V-shaped QWRs and studied the dependence of the electron ground state (E1) energy on the diffusion length. In this paper, we extend this study including the inter-diffusion effect on higher energy levels, as well as on the E1 wave function distribution.

## 2. Model and calculation details

A model V-shaped GaAs/$Al_{0.4}Ga_{0.6}As$ QWR grown in the (100) direction is considered. The central thickness of the crescent is 20 monolayers (MLs) (1ML=0.283 nm for (100) GaAs). Its cross section is obtained by two parabolas with curvatures corresponding to the curvatures taken from a TEM image of a real QWR. The bottom (upper) parabola curvature is $6.67 \times 10^{-3}$ ($3.62 \times 10^{-3}$) $ML^{-1}$, so the lateral width is about 150 ML (42 nm).

The inter-diffused interface concentration profile is calculated by Fick's second law, the diffusion length $L_D$ being a parameter determining the degree of the interface broadening [4]. To a first approximation, one-dimensional inter-diffusion (along the growth direction, $Y$) is considered. This is justified by the large difference between the vertical and lateral crescent dimensions. In the present calculations, $L_D$ is varied from 0 (abrupt interfaces) to 20 MLs. For larger $L_D$, two-dimensional inter-difusion should be taken into account.

To determine the bound state energies, a simple approach is applied, known as the adiabatic approximation for V-shaped QWRs [9,10]. It relies again on the fact that the crescent height is much smaller than its lateral width. So, the crescent is considered as being formed by several QWs (called "individual QWs") along $Y$, with different thicknesses. A given bound state energy level calculated for each individual QW builds up the shape of the lateral confinement potential well (along $X$), further called a "secondary QW". Thus, each level in the individual QWs gives rise to a series of levels, corresponding to the quasi-one dimensional confinement in the QWR. A simple one-band envelope function approximation (EFA) model is used in the calculations together with the material parameters from [11]. The EFA equation for each QW (individual or secondary) is solved numerically by the finite-difference method.

The area around the QWR is taken large enough to include the whole region, where the Al concentration for the maximum $L_D$ value changes by 2.5 % or more with respect to its initial value (0.4). Any smaller area leads to incorrect results about the bound state energies and wave functions.

## 3. Results and discussion

The central thickness of the crescent in this study is chosen to be $d$ = 20 MLs, because, as shown in [9], in the QWR with this thickness (and the same values of the other parameters) the first electron bound state energy level, E1, is strongly influenced by the inter-diffusion. Similar behaviour is also expected for the higher bound states energies. Figure 1 represents the calculated energies of the electron bound states as a function of $L_D$. The following general tendencies are observed: i) The bound state energies increase monotonically with increasing the interface grading (increasing $L_D$); ii) The increase is slow in the beginning, faster for intermediate $L_D$ values and reveals a saturation tendency at high $L_D$. Similar behaviour has been obtained for QWs in [5], where a detailed explanation is given. The third energy level undergoes a maximum increase when $L_D$ increases from 0 to 16 MLs. For large interface grading, the number of states localised in the QWR decreases, because the QW potential well becomes shallower.

It has been shown [12] that the shape of a rectangular QW subjected to inter-diffusion gradually changes to reach, at a given value of the diffusion length, a parabolic-like profile (in the central part), with equidistant levels. We have obtained a similar effect in the QWR under study. This is illustrated in Fig 2, which presents the energy levels from Fig.1, plotted as a function of the state number for different values of $L_D$. For $L_D$ = 0 ML (abrupt interfaces) the dependence is super-linear. This means that the levels are not equidistant, but their spacing increases with their increasing number, similarly to the case of a rectangular QW. With increasing $L_D$, the non-linear behaviour gradually changes toward a linear one, and for $L_D$ > 14 MLs the QWR levels become practically equidistant. This is a consequence of the fact that with increasing $L_D$ the shape of the secondary QW potential increasingly approaches a parabolic shape, as shown in the inset of Fig.2. The transition towards equidistant energy levels with increased interface grading in a V-shaped QWR, which is a more complicated structure than a QW, is an interesting effect that could find various applications.

Furthermore, the first electron state wave function is calculated for different diffusion lengths. Figure 3 shows contour plots of the normalized (to ten) squared wave function two-dimensional profile $\Psi^2(X,Y)$ for $L_D$ = 0, 8 and 20 ML.

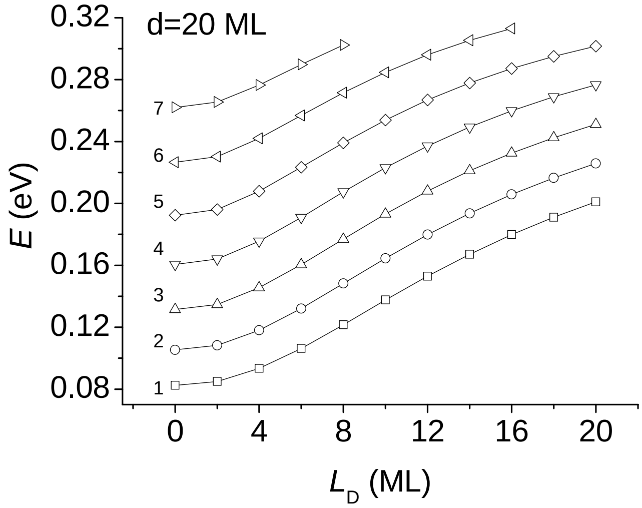

*Fig.1 Electron bound states energies of a 20ML thick QWR as a function of the diffusion length.*

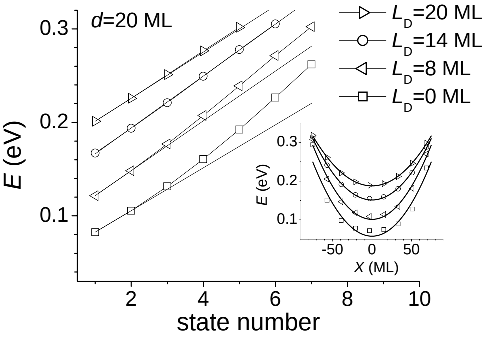

*Fig. 2. Electron bound states energies versus the state number for different values of $L_D$. The straight lines demonstrate the deviation from linear dependence. The inset shows the corresponding secondary QW profiles fitted to parabolas.*

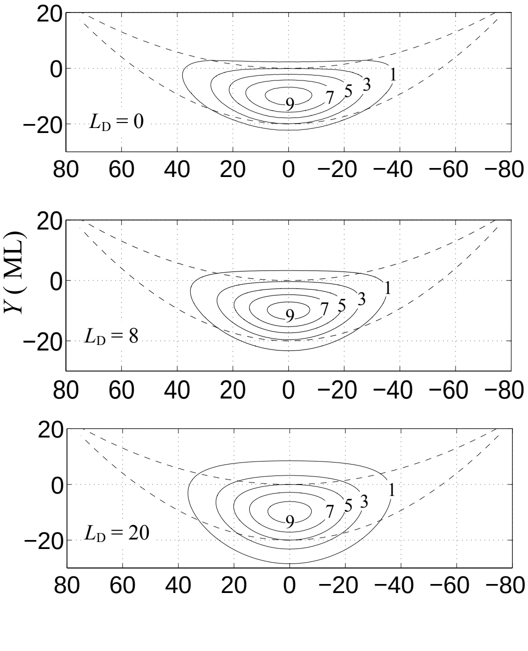

*Fig. 3. Contour plots o ɔ ten) squared wave function two-dimensional profile $\Psi^2(X,Y)$ for $L_D$ = 0, 8 and 20 ML. The dashed lines represent the QWR contours at $L_D$ = 0 ML.*

For a quantitative description of the wave function localization, we focus on two parameters, called $W_X$ and $W_Y$. They are defined as the full-width-at-half-maximum (FWHM) of $\Psi^2(X,Y)$, measured along the $X$ and $Y$ directions, respectively. In the QWR with abrupt interfaces, $W_X$ = 42.7 ML and $W_Y$ =15.7 ML, i.e. the E1 state is localized predominantly in the QWR potential well (Fig. 3a). Figures 4 and 5 present the dependences of $W_X$ and $W_Y$, on the diffusion length. For small $L_D$ values, both parameters decrease to reach a minimum and then increase again. $W_X$ has a minimum of 38.8 ML at $L_D$ = 12 ML, while the minimum of $W_Y$ is 14.5 ML and occurs at $L_D$ = 6 ML. At $L_D$ =20 ML, the value of $W_X$ (40.2 ML) is lower than that corresponding to abrupt interfaces ($L_D$=0 ML), while $W_Y$ reaches 20 ML, which is essentially larger than its initial value. The dependence of $W_X$ and $W_Y$ on the diffusion length is also shown in Fig. 6, as a parametric plot. In the figure, the ($W_X$ ,$W_Y$) point labelled $L_D$=0 ML gives an idea about the wave function expansion in the initial QWR with abrupt interfaces, while that labelled $L_D$ = 20 ML corresponds to the QWR with maximum inter-diffusion.

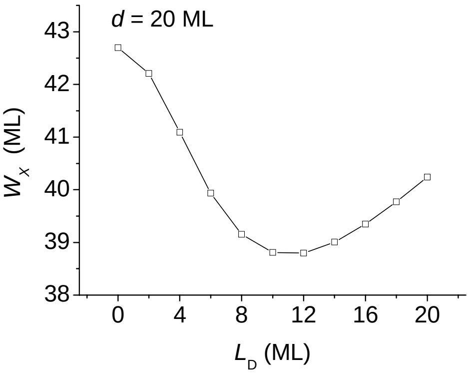

*Fig. 4. FWHM along X of the normalized squared wave function of state E1.*

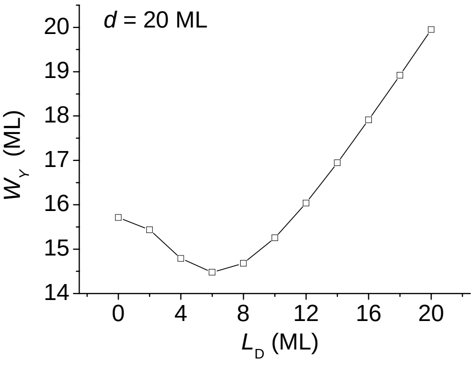

*Fig.5. FWHM along Y of the normalized squared wave function of state E1.*

We emphasize the following points:

i) Contrary to its energy, the wave function of the E1 bound state reveals non-monotonic behaviour with increasing the diffusion length, as can be seen in Figs.3, 4 and 5. The decrease of $W_X$ and $W_Y$ corresponds to an increasing localization of the E1 state, while the increase of $W_X$ and $W_Y$ corresponds to its delocalization.

ii) It is interesting to note that the stronger localization along $X$ and $Y$ occurs at different $L_D$ values. This means that in a range of $L_D$ values between 6 and 12 ML the wave function already expands along the growth direction, but still shrinks along the lateral one. Therefore there is no $L_D$ value that leads to a minimum of both $W_X$ and $W_Y$. However, as the change of $W_Y$ is quite small (only ~1 ML) for 0 < $L_D$ < 6, the best localization is achieved at $L_D$ = 8-10 ML, as seen from Fig. 6.

iii) After $L_D$ = 12 ML, the wave function expands in both directions, but much faster along $Y$. At $L_D$ =20 ML, a considerable part of $\Psi(X,Y)$ extends outside the initial QWR along the growth direction. As to the lateral direction, the net result of the inter-diffusion with $L_D$ = 20 ML is compression of the wave function ($W_X$ ($L_D$ = 20 ML) < $W_X$ ($L_D$ = 0 ML)), as revealed by Figs. 3 and 6. This is a consequence of the fact that the potential in the crescent edges grows faster with $L_D$ compared to that in the crescent centre, because of the different widths of the individual QWs.

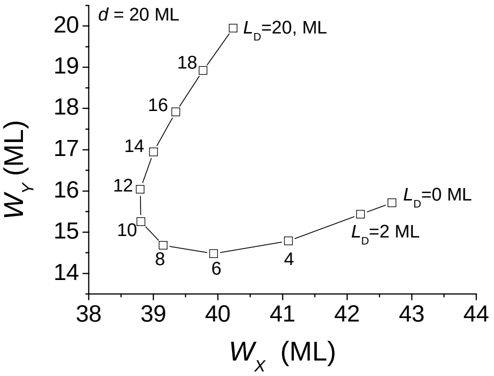

*Fig. 6. Parametric plot of $W_X$ versus $W_Y$, with the diffusion length as a parameter.*

## 4. Conclusions

We have modelled the inter-diffusion in a 20 ML thick V-shaped GaAs/$Al_{0.4}Ga_{0.6}As$ QWR and studied its influence on the electron state energies and wave functions. The electron state energies increase monotonically with the diffusion length, with a tendency to become equidistant. At the same time, the ground state wave function changes non-monotonically: it initially shrinks slightly, which is followed by a strong expansion in the growth direction. Although the maximum compression does not occur simultaneously along $X$ and $Y$, there is a range of diffusion length values (8-10 ML) corresponding to relatively good wave function localization. The results obtained contribute to the elaboration of a technological procedure for controllable spatially selective tuning of the QWR optical properties to achieve integrated photonic devices.

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