Shallow impurities in V-groove quantum wires

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(Received 5 May 2000; revised manuscript received 19 October 2000; published 1 March 2001)

We calculate the binding energies for shallow impurities in V-groove GaAs/$Al_xGa_{1-x}As$ quantum wires using a variational technique. The carrier ground states are calculated by an effective potential method together with a suitable coordinate transformation that allows the decoupling of the two-dimensional wave function. This method enables a detailed calculation of binding energies, providing an efficient tool for the study of impurity-related properties in V-groove wires. We show that the lateral confinement of the V-groove potential localizes the impurity wave function very effectively in the central region of the quantum wire.

DOI: 10.1103/PhysRevB.63.113307 PACS number(s): 71.55.Eq, 73.20.Hb, 73.21.−b, 71.38.−k

The electronic and optical properties of quantum wires have attracted increasing attention recently. Several growth techniques have been successful in obtaining a type of heterostructure known as V-groove or ridge quantum wires. These V-groove quantum wires have been obtained for a variety of materials such as $In_yGa_{1-y}As/GaAs$,[1] $In_yGa_{1-y}As/Al_xGa_{1-x}As$,[2] $In_yGa_{1-y}As/InP$,[3] $In_yAl_{1-y}As/InP$,[4] $GaAs/Al_xGa_{1-x}As$,[5–7] and Si/SiO_2.[8] Certainly, to fully understand the optical and electronic properties of V-groove quantum wires, a description of the impurity properties would be important.

The calculation of shallow impurities in square and circular quantum wires is currently well established.[9–12] However, the variational technique employed for the calculation is numerically intensive if the wire is not of circular shape. Due to the complicated form of the potential profile in V-groove quantum wires the calculation of shallow impurity states may become impractical if the method of calculation of the carrier ground states is also numerically intensive. Several theoretical approaches have been put forth for the calculation of the energy levels and wave functions: Sa'ar *et al.*[13] proposed a local-envelope states expansion, Pescetelli *et al.*[14] used a tight-binding approach for T- and V-shaped quantum wires, and Ammann *et al.*[15] used a quasifactorization scheme. However, in general the two-dimensional effective mass Schrödinger equation has been calculated numerically using either plane-wave expansion[16–20] or by adapting finite element methods.[21]

A detailed calculation of shallow impurity states in V-groove quantum wires, to the best of our knowledge, is still not available. For experimental studies of V-groove quantum wires it is important to have a theoretical description of the impurity levels in addition to other physical properties. For instance, for the study of photoluminescence spectra it is important to be able to identify the observed peaks as impurity related or rule them out as such. The presence of additional structures, such as vertical quantum wells and pinch-off regions, adds new energy states to an already complicated spectrum, emphasizing the necessity of a complete level structure calculation. For calculations of impurity-related optical properties, such as impurity absorption coefficients and photoluminescence spectra, a detailed knowledge of the impurity binding energy is needed over all spatial regions of the quantum wire. A partial knowledge, e.g., of a few symmetry points, is not sufficient for this purpose. This calls for a theoretical model that should be numerically very efficient.

In this work we use an effective potential method, proposed in Ref. 22, that allows the decoupling of the two-dimensional wave function of the V-groove quantum wire.[13–21] The purpose of this paper is to obtain the shallow impurity binding energies and to establish how effectively the shallow impurity responds to the lateral confinement of a V-groove quantum wire. This method provides energy levels and wave functions that are in agreement with more complicated calculations. Also, it is numerically efficient and thus provides an important tool for the study of impurity-related phenomena in V-groove quantum wires. Furthermore, it is a direct application of the effective potential method[22] allowing us to further assess the validity of this method of calculation.

We first write the Hamiltonian for a Coulombic shallow impurity,

$$H = H_0 - \frac{e^2}{\epsilon[(x-x_i)^2+(y-y_i)^2+z^2]^{1/2}}, \tag{1}$$

where

$$H_0 = -\frac{\hbar^2}{2m^*}\nabla^2 + V(x,y) \tag{2}$$

is the Hamiltonian without the impurity potential.

To calculate the carrier ground state we assume the following potential profile to describe the interface potentials of the V-groove quantum wire:[21,22]

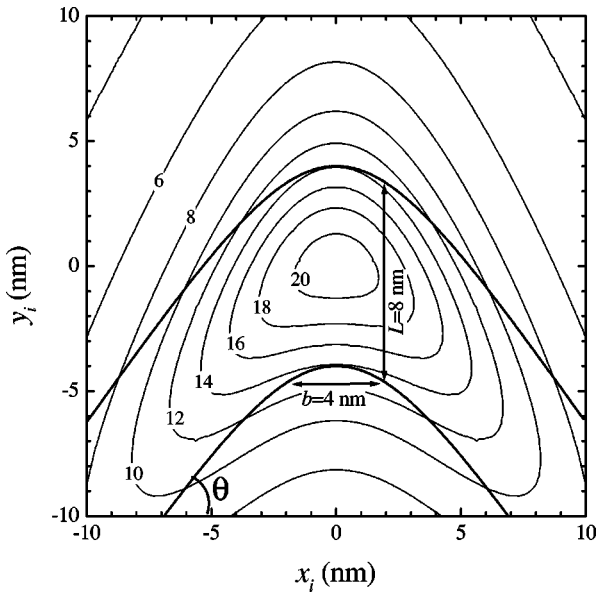

FIG. 1. Calculated donor binding energies as a function of the impurity position x_i and y_i. The contour plots show curves with the same binding energy listed in meV (number displayed at each curve). The V-groove quantum wire dimensions are $b=4$ nm, $L=8$ nm, and angle $\theta=54.75°$.

$$y_1(x) = -b \tan\theta \ln[\cosh(x/b)] + \frac{L}{2}, \tag{3}$$

$$y_2(x) = y_1(x) - L, \tag{4}$$

where L is the channel width along the y direction and b represents the bend width at the top of the ridge (see, for example, Fig. 1). Here we have defined the angle θ such that $180° - 2\theta$ is the angle between the facets of the ridge, the angle normally referred to in most articles. We then apply the coordinate transformation[21,22]

$$X = x, \tag{5}$$

$$Y = -y - b \tan\theta \ln[\cosh(x/b)], \tag{6}$$

$$Z = z \tag{7}$$

to the Hamiltonian H_0. In the transformed coordinates the potential barrier becomes linear and resembles that of a simple quantum well, i.e., it becomes a function of Y only. The transformed Hamiltonian H_0 becomes considerably more complicated as it now contains all the information about the lateral confinement.[22] Our approximation consists of replacing all mixed terms of the transformed Hamiltonian by an effective lateral potential[22]

$$V_{\text{eff}}(X) = V_X \tan\theta \tanh^2(X/b), \tag{8}$$

where V_X is an angle-independent barrier factor. This potential allows the decoupling of the two-dimensional Hamiltonian into two readily solved one-dimensional Hamiltonians.

The impurity binding energy is calculated using a standard variational technique; for details see Refs. 9, 23, and 24. The trial wave function is chosen as

$$\psi(X,Y,Z) = N\phi(X,Y)\exp\{-[(X-X_i)^2 + (Y-Y_i)^2 + Z^2]^{1/2}/\lambda\}, \tag{9}$$

where X_i, Y_i is the impurity position in transformed coordinates, and λ is the variational parameter. $\phi(X,Y)$ is the ground state wave function without the impurity, i.e., the eigenfunction of H_0 obtained in transformed coordinates. All calculations are carried out in transformed coordinates. The binding energy $E_B = E_0 - E$ is obtained by numerically minimizing the energy E with respect to the variational parameter λ, where E_0 is the ground energy level without the impurity.

We present results for GaAs/$Al_{0.3}Ga_{0.7}$As V-groove quantum wires and we discuss the binding energies for donor impurities as a function of impurity position in the wire. We used an effective mass for GaAs of $0.067m_0$ and a dielectric constant of $13.18\epsilon_0$.[25] The barrier height is 264 meV for the conduction band.[21] Also, we use a barrier factor V_X of 42.4 meV for the conduction band.[22] The angle is $\theta = 54.75°$ such that $180° - 2\theta$ corresponds to the measured angle between the two facets of the ridge.[21,22] For comparison we also consider a smaller angle (larger angle between the facets) of $\theta = 30°$, since we notice that for multiple V-groove quantum wires the angle between the facets $(180° - 2\theta)$ becomes increasingly larger (e.g., Ref. 7).

The donor binding energies as a function of the impurity position x_i and y_i are presented in Fig. 1 for a V-groove quantum wire with channel width of 8 nm and bend width of 4 nm. The binding energies are clearly consistent with a two-dimensional confinement in the central region of the quantum wire. Note that the binding energy is maximum for a donor located at the center of the V-groove quantum wire and decreases continuously as the donor position is moved away from the center. A larger decrease is observed for donors located in the barrier region. This behavior can be understood by analyzing the impurity wave function. Figure 2 shows the wave function for several impurity position in the quantum wire. For an impurity located at the center of the wire [Fig. 2(a)] the wave function is clearly *s*-like and as such has the largest possible binding energy. For impurities located at the interface [Figs. 2(b) and 2(c)], but still within the central region, the wave function becomes strongly deformed, thus giving smaller binding energies. As we move the impurity along one of the wings of the V-groove wire [Fig. 2(d)] away from the central region the wave function becomes even more deformed, thus accounting for smaller binding energies.

We discuss now the dependence of the donor binding energy on the V-groove quantum wire dimensions. We consider two situations as compared to the quantum wire shown in Fig. 1: a smaller angle to consider a smaller lateral confinement and a smaller channel width to consider a larger confinement. For a smaller angle $\theta = 30°$ as shown in Fig. 3(a) we observe smaller binding energies in agreement with a smaller lateral confinement. The limit situation of $\theta = 0$, i.e., a simple quantum well of the same width (8 nm), has a

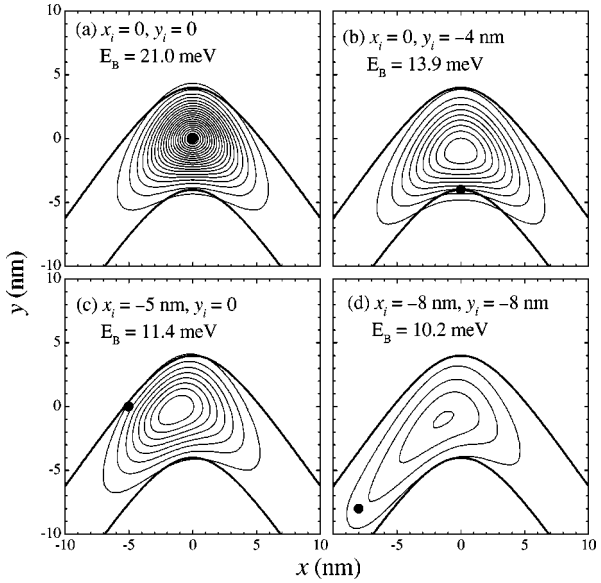

FIG. 2. Contour plots of the impurity wave function $\psi(x,y,z=0)$ in arbitrary units. The V-groove quantum wire has dimensions $b=4$ nm, $L=8$ nm, and angle $\theta=54.75°$. Four different impurity positions, each marked with a full circle, are shown in parts (a) to (d).

donor binding energy at its center of 12.8 meV.[26] Figure 3(b) shows a wire with smaller channel width, where we find binding energies up to 23 meV. Note that this binding energy is larger than for the wire in Fig. 1. This is explained as follows. Both wires have the same structural parameters, the only difference being a narrower channel width in Fig. 3(b). Thus with a larger confinement of the wave function we obtain also a larger binding energy. These two situations shown in Fig. 3 demonstrate that the effective potential used for calculating the binding energies provides consistent and reliable results. Also, the overall behavior of the impurity binding energy calculated with the effective potential is in agreement with several results for quantum wires of different shapes.[9–12]

A recent paper by Deng *et al.*[27] also presents calculated donor binding energies in V-groove quantum wires at some specific impurity positions. These authors present binding energies for three impurity positions, which are comparable to our results for the same wire positions.

In conclusion, we calculated shallow impurity binding energies in V-groove quantum wires using an effective potential method for the calculation of the electron and hole ground states. Our results show that the lateral confinement is very effective and that the impurity wave functions become strongly localized in the central region of the V-groove quantum wire. The calculated binding energies are comparable to those obtained for circular or rectangular quantum wires.

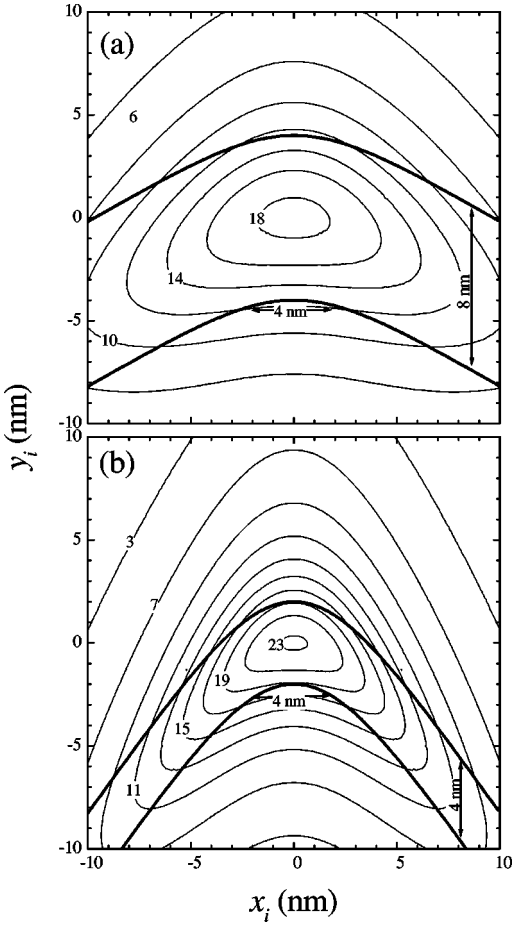

FIG. 3. Contour plots of the donor binding energy in V-groove quantum wires with dimensions (a) $b=4$ nm, $L=8$ nm, and angle $\theta=30°$ and (b) $b=4$ nm, $L=4$ nm, and $\theta=54.75°$.

We are grateful to G. Creci for helpful discussions, and acknowledge financial support from CNPq (Grant Nos. 522789/96-0 and 300917/91-0), Fapesp (Grant No. 96/10871-1), and PEPCI/USF.

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