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Theory of electronic and optical properties for different shapes of $InAs/In_{0.52}Al_{0.48}As$ quantum wires

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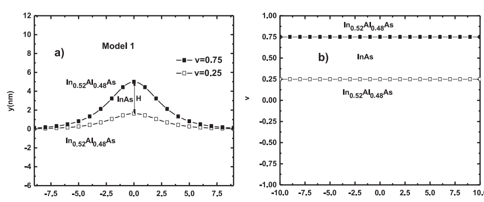
HIGHLIGHTS

- We are interested for $InAs/In_{1-x}Al_x$ As quantum wires.
- We present a method for energy spectra and wave function calculations.
- The method is based on the coordinate transformation.
- The influence of the parameters introduced is studied on the optical properties.

GRAPHICAL ABSTRACT

We have used an efficient method based on the coordinate transformation for numerical modeling of different shapes of quantum wires.



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ABSTRACT

In this work, we propose an efficient method to investigate optical properties as well as their dependence on geometrical parameters in InAs/InAlAs quantum wires. The used method is based on the coordinate transformation and the finite difference method. It provides sufficient accuracy, stability and flexibility with respect to the size and shape of the quantum wire. The electron and hole energy levels as well as their corresponding wave functions are investigated for different shape of quantum wires. The optical transition energies, the emission wavelengths and the oscillator strengths are also studied.

1. Introduction

Due to current growth techniques of semiconductor nanostructures, different shapes of quantum wires have been obtained in a variety of materials such as InAs/InP [1], GaAs/AlGaAs [2] and InGaAs/GaAs [3]. Thus, considerable mathematical efforts have been deployed by scientists to model and simulate such different shapes of nanostructures. The main used equation is the Schrödinger equation resolved with finite difference method (FDM). We have used this theoretical approach in our past works in the case of rectangular quantum wires [4] and cubic quantum dots [5]. Despite the obtained good results, this method is limited to simple

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geometric problems. Thus, many authors have concentrated their studies on the techniques of analytical and numerical resolution. Pescetelli et al. [6] have used a tight-binding approach for T-and V-shaped quantum wires while Greci and Weber [7] have used the coordinate transformation, they have obtained a planar interface and they have decoupled analytically the 2D Schrödinger equation, each direction is thus resolved numerically.

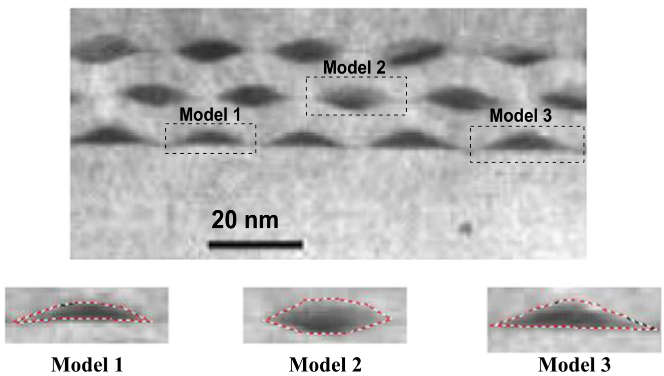

Fig. 1. TEM picture of closely stacked InAs quantum wires in InAlAs matrix.

In the present work, our purpose is the modeling of InAs/InAlAs quantum wires and the investigation of their electronic and optical properties. These structures are used in long-wavelength semiconductor laser diodes (1.55 μm) and infrared photodetectors [8]. Many experimental works have shown that the InAs nanostructures are grown on In0.52Al0.48As/InP substrate using molecular beam epitaxy. The 3% lattice mismatch characteristic of this material system, allows full coverage of the surface with either quantum wires or elongated quantum dot. The works of Fossard et al. [9] and Weber [10] demonstrate that the system of InAs/InAlAs, quantum wire and elongated quantum dot have same properties and they are very similar.

They also have the particularity to offer several shapes, for same sample and for different layers, as mentioned in the works of Lin et al. and Wang et al. [11,12] and shown in Fig. 1 [11]. The theoretical method proposed to model complex forms of quantum wires, is based on the coordinate transformation. It makes simpler the geometry of the structure leading to flat interfaces of the structure and computational domain, and enabling implementation of the FDM within a new coordinate space. We have used this method recently to investigate the electronic and optical

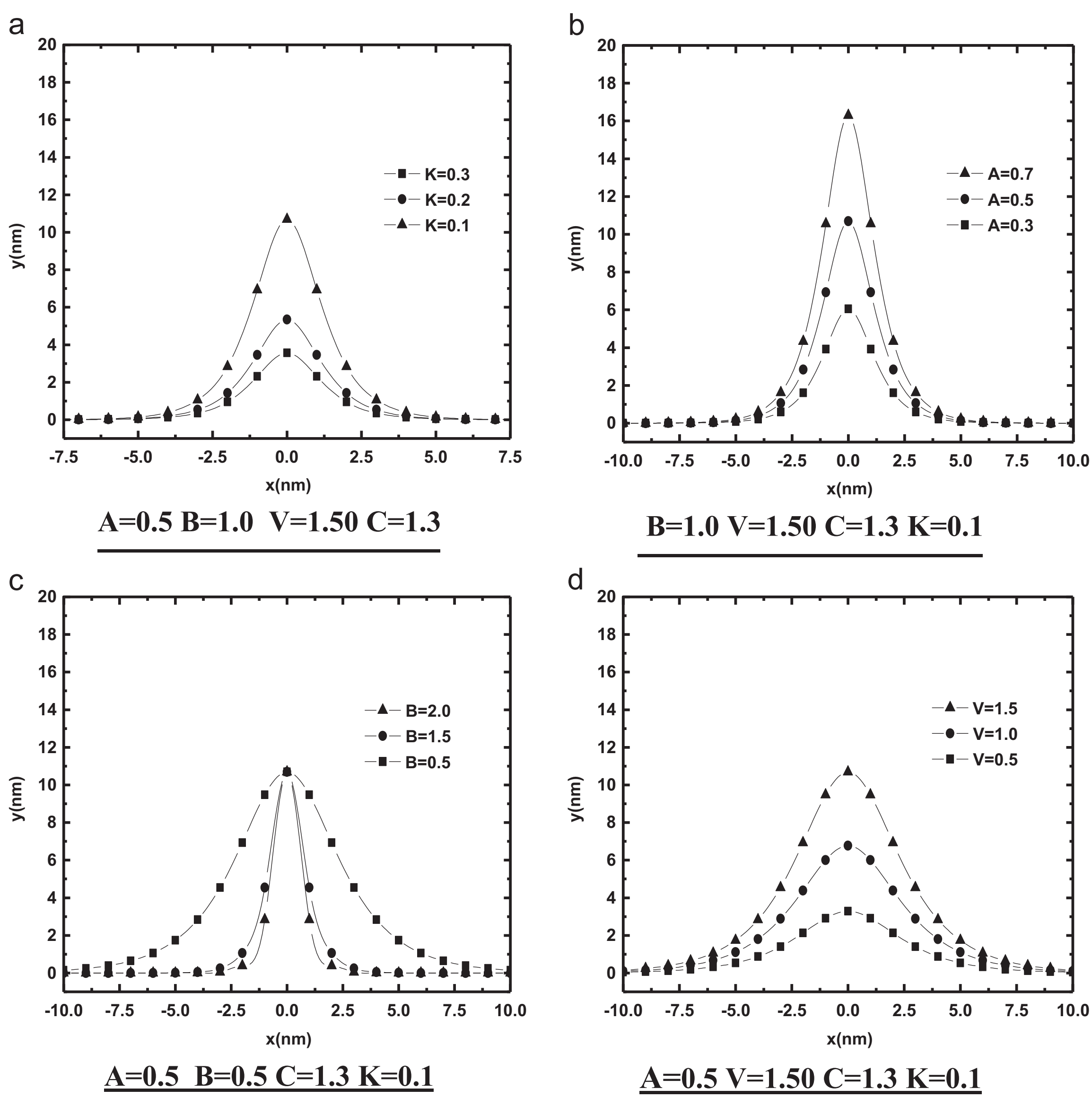

Fig. 2. The effects of parameters K a), A b) B c) and v d) on the shape of the quantum wire.