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Charge redistribution induced by donors in nanowires with variable composition and thickness

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ABSTRACT

By using the functional derivative technique we study the binding energies of on- and off-axis donors in compositionally modulated nanowires and in nanowires with variable thickness and different profiles of the cross-sections along the axis, in the presence of the external electric field applied parallel to the growth direction. We show that the electronic properties of donors in narrow non-homogeneous wires are very sensitive to the variation of their positions, the heterostructure geometry and the composition. Binding energy dependencies on the electric field strength, the barrier and well widths, the wire radius, as well as the donor position are consistently described using our formulation. Our simple method should be useful for analyzing a variety of more complex nanowire superlattice structures and nanowires with variable cross-section profiles, for which more rigorous approaches require extensive numerical calculations.

1. Introduction

One-dimensional (1D) nanostructures such as wires, rods, belts, and tubes are currently the subject of intense research owing to their unique applications in mesoscopic physics and fabrication of nanoscale devices. In comparison with quantum dots and wells, the advancement of 1D nanostructures has been slow until very recently, as hindered by the difficulties associated with the synthesis and fabrication of these nanostructures with well-controlled dimensions, morphology, phase purity,

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and chemical composition. But unconventional methods based on chemical synthesis, elaborated in the last decade, have provided an alternative and intriguing strategy for generating 1D nanostructures in terms of material diversity, cost, throughput, and the potential for high-volume production [1].

Advances in manufacturing of 1D nanostructure materials have allowed, particularly, the growing quasi-one-dimensional compositionally modulated heterostructures [2] which are known as nanowire superlattices (NWSLs). These structures can be successfully fabricated using various growth techniques most of which are based upon a nanocluster catalyst. Today, NWSLs are the subject of intense research since these are expected to have a wide range of future applications such as nanobar-codes, nanolasers and light-emitting diodes. Because the electrical and optical properties of NWSLs are defined by the interplay between the confinement of the particles, tunnelling through the barriers between neighbouring wells and the interaction between particles, these structures may show better characteristic properties as compared to nanowires [3] due to the coupling of the superlattice longitudinal confinement to the nanowire radial confinement. One can expect that such coupling opens up new opportunities for controlling the charge distribution and the spectrum of NWSLs by varying their composition or geometry. Depending on these characteristics, the structure may have properties similar to quantum dots (QD), quantum wells (QW), quantum well-wires (QWW) or superlattices (SL). For example, when the radius of the NWSL is very large its electronic properties are similar to those of SL, for small radii they are similar to those of the QWW, while for intermediate values of the radius they should be similar than those of the QD or the QW. The smaller the NWSL radius, the stronger the radial confinement, the higher energy levels, and the more extended the electronic states are due to the stronger tunnelling through the barriers along the axis.

The effect of the confinement on the energy spectrum and the charge distribution in NWSLs with a single electron has been studied previously by using different numerical methods [4]. The effect of the confinement on the neutral D^0 and negatively charged donors in NWSLs has been studied recently [5] by using the Fractional Dimensional Method, elaborated previously for solving this type of problem in heterostructures [6]. Nevertheless, the infinite barrier model, used in Ref. [5] ignores the possibility of the electron tunnelling outside the NWSL structure in the radial direction, the process that becomes significant as the NWSL radius is small. Besides, the model considered in Ref. [5] disregards a possible variation of the wire thickness that may be significant in the really fabricated nanowires [1]. Such variations in a narrow NWSL can provide a significant decrease of the differences between energies in the wells and barriers making possible a stronger electron tunnelling along the axis. Therefore one can expect that narrow NWSLs should have different electronic properties from those of other types of nanostructures, which in addition may be controlled much easier by varying the geometry of the cross-section or the nanowire composition. It is motivation for presenting below the extension of the analysis of electronic properties of donors confined in a periodic NWSL presented in the paper [5] considering a model with finite-barrier lateral confinement and possible variable thickness.

2. Theoretical framework

In this model the GaAs/$Ga_{1-x}Al_xAs$ NWSL is embedded in the $Ga_{1-y}Al_yAs$ matrix. The NWSL has circular cross sections with a variable along the growth direction z Al concentration $c(z)$ or radii $R(z)$. In the first case, such a structure we call the compositional NWSL and in the second case the structural NWSL. In Fig. 1(a) we present a scheme of a compositional NWSL in which the Al concentration is equal to zero inside 5 identical wells of the width a, to x in the 4 barriers of width b and to y outside the NWSL and in Fig. 1(b) a scheme of a structural NWSL with periodically variable radius $R(z)$. In our calculations we assume that the confinement potential $V(\rho, z)$ in cylindrical coordinates provided by discontinuities of the conduction band bottom in junctions, is related to respective discontinuities of the Al concentration distribution $c(\rho, z)$ by means of the formula $V_c(\rho, z) = 0.6[1.36c(\rho, z) + 0.22c^2(\rho, z)]$ (eV) [7]. To analyze the properties of compositional NWSLs we consider a model in which the Al concentration $c(\rho, z)$ is equal to $c(z)$ inside the NWSL where $0 < \rho < R(z)$ and to y otherwise. To simulate the structural NWSL we assume that confinement potential $V(\rho, z)$ is equal to zero as $0 \leq \rho \leq R(z)$ and to infinity otherwise. For the sake of mathematical convenience, in this work we do not consider the effect of the dielectric confinement [9], assuming that the dielectric constant mismatch at the junctions is depreciable.