Localization of Electron and Hole Gas in Hexagonal Core-Multishell Nanowires

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INTRODUCTION

Multishell coaxial semiconductor nanowires are attracting much interest due to their possible application as light harvesting devices[1], nanophotonic sources [2], and nanoscale FETs with novel geometries[3]. The cross-section of low-impurity nanowires usually reflects the prismatic crystallographic arrangement and can hardly be considered circular. In particular, III-V nanowires often show an hexagonal shape, with the embedded curved 2DEG wrapped on the surface of the prismatic hexagonal interface between different materials. The inclusion of the 2DEG shape in the calculation of electronic states is thus of primary importance since it leads to localization of carriers on the corners of the hexagon[4]. Here, we study how the self-consistent band profile induces the formation of shallow channels for electrons along the edges, and show how the system geometry and doping profile tailor the mutual coupling of such 1D regions.

SYSTEM LAYOUT

We consider a prismatic nanowire with hexagonal cross section[5,6]. The internal GaAs core is covered with a 7 nm AlAs uniform layer and another 13.5 nm GaAs layer as shown in Fig. 1. A thin layer of n dopants with density $5\text{x}10^{25}$ part/m^3 (nominally a delta-layer doping) is introduced in the middle of the AlAs region. Fermi level is pinned to the middle of the gap on the external surface. The results presented are obtained for a temperature of 4 K.

NUMERICAL APPROACH

To obtain the self-consistent electronic states we solved iteratively the closed 2D Schrödinger and Poisson equations for electrons and holes on the hexagonal domain. In order to avoid spurious effects from the mismatch between a rectangular grid and the shape of the domain we developed software codes for the above equations relaying on the box-integration method with hexagonal boxes. This allows a straightforward inclusion of both the Dirichlet and Neumann boundary conditions on the domain edges, since they are aligned with the box edges.

RESULTS

We find different localization regimes for electrons and holes[7]. In particular, conduction-band electrons form six 1D channels along the corners, whose mutual coupling can be tailored by the sample geometry and doping density.

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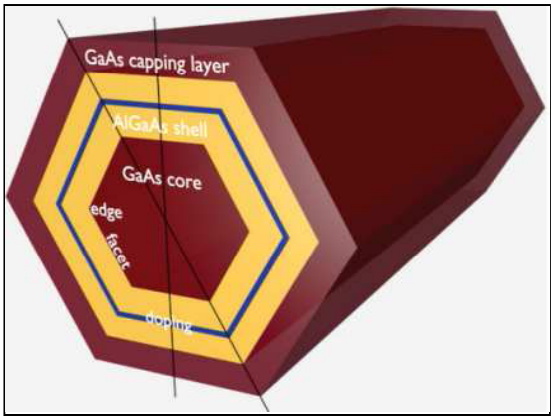

Fig. 1. Geometry and composition of the sample cross-section. The edge of the hexagonal cross-section is 66 nm.

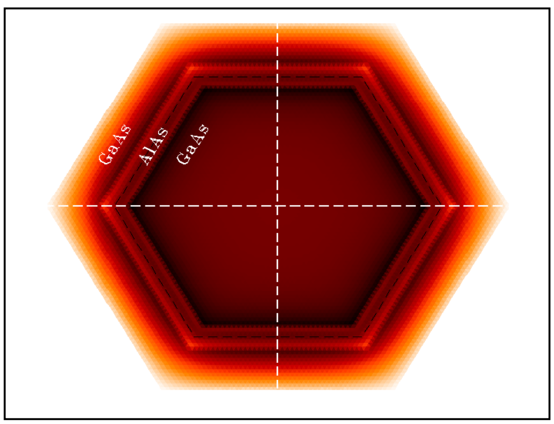

Fig. 2. Self-consistent conduction-band profile. Darker color indicates a lower energy. The two dashed lines represent the two sections shown in Fig. 4.

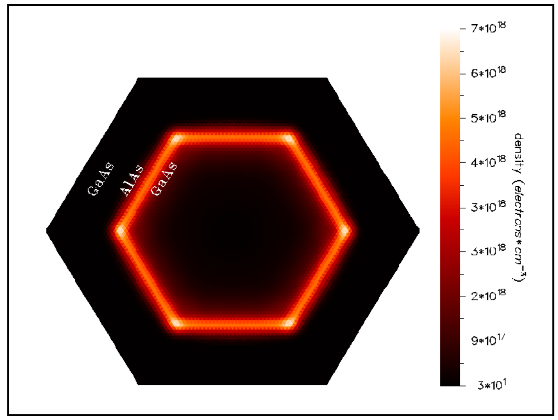

Fig. 3. Self-consistent electron density. Six channels are formed on the corners of the AlAs-GaAs interface.

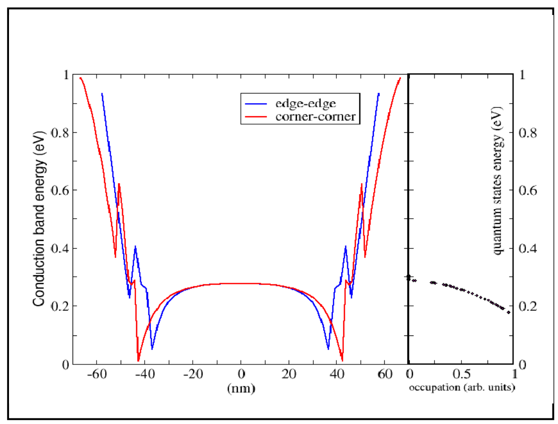

Fig. 4. Self-consistent conduction band along the horizontal (red) and vertical (blue) directions as shown in Fig. 2. Triangular wells are formed at the AlAs-GaAs interface. The localization on the edges is stronger. On the right, the energy and occupation of the first 70 quantum levels is reported. Due to the shape of the system many degenerations are present.