Self-consistent k.p band structure in doped core-shell nanowires with type-I, type-II and broken-gap radial heterointerfaces.

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INTRODUCTION

Tailoring spin-orbit coupling and valence-band mixing in nano-fabricated semiconductors is critical to engineer scalable spintronic devices. Here, we present our numerical investigations on the electronic band structure of modulation-doped GaAs/AlGaAs and InAs/GaSb core-shell nanowires (CSNW) with both *n*- and *p*-type doping. Calculations are performed by a recently developed self-consistent finite-element library able to treat a broad class of CSNWs which will be described.

MODEL AND METHOD

We adopt an 8-band Burt-Foreman $k \cdot p$ Hamiltonian approach which describes coupled conduction and valence bands in heterostructured nanowires of arbitrary radial composition, growth directions, and doping. Coulomb interactions with the electron/hole gas are taken into account within a mean-field self-consistent approach. We map the ensuing multi-band envelope function and Poisson equations to optimized, nonuniform real-space grids (fig. 1). Self-consistent charge-density, single-particle subbands, density of states, and absorption spectra are obtained at different doping regimes[1]. We extend previous investigations to realistic descriptions of modulation-doped samples. The use of a flexible numerical approach, with nonuniform grids, proved to be critical to treat doping levels at comparable numerical loads.

RESULTS

For *n*-doped Gas/AlGaAs samples, a large restructuring of the electron gas for increasing doping takes place and results in the formation of quasi-1D electron channels at the core-shell interface (fig. 2). For *p*-doped samples, strong heavy-hole/light-hole coupling of valence states leads to non-parabolic dispersions with mass inversion (fig. 3), similar to planar structures, which persist at large doping, giving rise to both heavy-hole and light-hole gaps. In addition, the hole gas forms an almost isotropic, ringlike cloud for a large range of doping. We will also show that signatures of the evolution of the band structure can be singled out in the anisotropy of linearly polarized optical absorption[1].

In InAs/GaSb CSNWs a type-II/broken gap alignment transition takes place, which changes the topological nature of the gap, depending on structural parameters[2,3], making this system a building block for topological quantum gates and for non-abelian physics. Based on our library, we propose a numerical protocol to calculate the self-consistent charge in broken-gap materials, where band alignment induces charge transfer also at charge neutrality. Therefore, we are able to expose the role of the self-consistency field in assessing the metallic or semiconductor character of the nanostructure (fig. 3) and driving the topological transition both by structural parameters and external gates.

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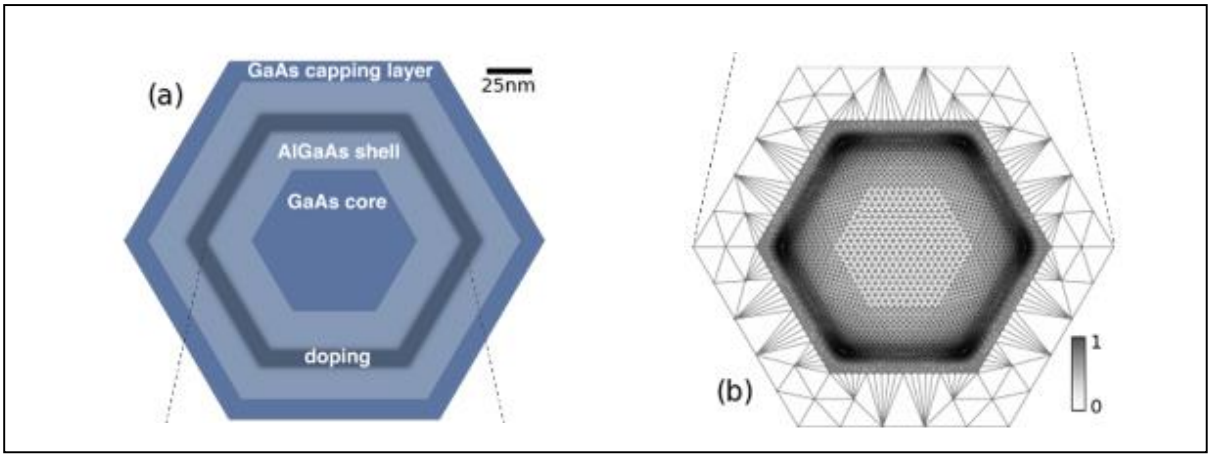

Fig. 1. (a) Cross-section of the GaAs/AlGaAs CSNW illustrating the different materials and the doped region. (b) Example of an optimized FEM grid used to solve the k.p equation of motion with superimposed self-consistent charge density (in grey scale arbitrary units). The grid is limited to the core and first shell, as indicated by the dashed lines.

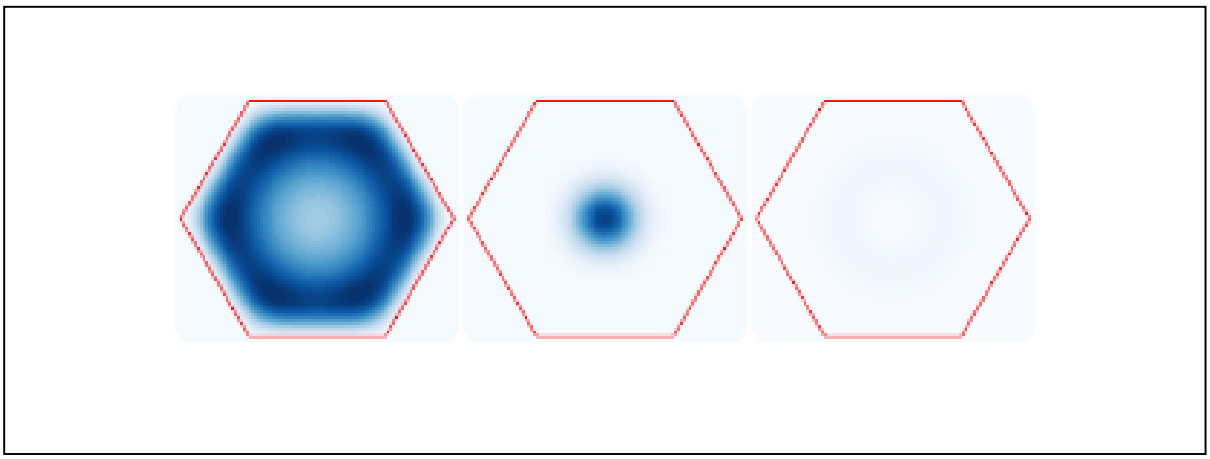

Fig. 2. Electron (left), light-hole (center) and heavy-hole (right) density for the ground of a heavily doped GaAs/AlGaAs sample, with doping density 1.9×10^{18} cm^{-3} .

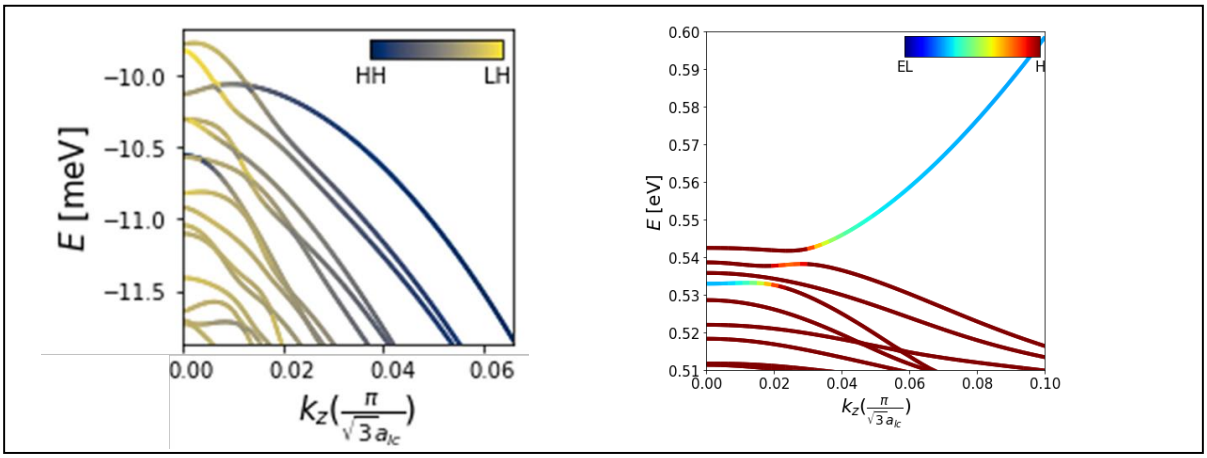

Fig. 3. Left: valence bandstructure of a GaAs/AlGaAs sample with doping density 1.73×10^{18} cm^{-3} showing mass inversion. Right: Bandstructure of a InAs/GaSb sample showing band hybridization and the opening of an energy gap induced by the spin-orbit coupling and the self-consistent field. The color respectively indicates the weight of the heavy/light hole or electron/hole character of the states.