Charge confining mechanisms in III-V semiconductor nanowires

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***Abstract*—III-V semiconductor nanowires exhibit unique features for application in novel optoelectronic devices. Due to their large surface-to-volume ratio, the realization of heterostructures beyond the capabilities of planar growth, that can still be integrated in Si-based electronics, becomes possible. Furthermore, polytypism was observed e.g. in GaAs nanowires such that different crystal phases coexist in the same nanowire. As different crystal phases have different electronic properties, this feature can be exploited to form crystal-phase heterostructures with atomically flat interfaces and only very small elastic deformation. We will discuss the specifics of electronic-structure simulations in such nanowires and present recent example studies.**

I. INTRODUCTION

Nanowires consisting of compound semiconductor materials have attracted much research interest in the past as they facilitate the realization of nanostructures for applications in modern electronics for which quantum dots or planar systems appear unsuited. For example, it is possible to produce compositional heterostructures even from materials which exhibit a large lattice mismatch, with dislocation-free strain relaxation being possible via the free side facets. The alloy compositions that can be achieved in nanowires are unattainable in planar systems, spanning a wide spectral range e.g. for light emitting or detecting devices [1].

Generally, compositional heterostructures can be produced in axial (e.g. (In,Ga)N disks in GaN nanowires) or radial (e.g. (In,Ga)As/GaAs core-shell nanowires) directions where the above advantages apply. Another very specific feature of semiconductor nanowires is that the coexistence of different crystal phases is commonly observed. In GaAs nanowires, segments of the zincblende and the metastable wurtzite phase are regularly seen. Simulations of elastic, piezoelectric, and optoelectronic properties are a significant part of the design process of semiconductor nanowires. Given the comparatively large size of realistic nanowire heterostructures, continuum models such as continuum elasticity and multiband $\mathbf{k}\cdot\mathbf{p}$ models, appear to be the best choice for accurate and computationally inexpensive simulations. In particular, the six- and eight-band $\mathbf{k}\cdot\mathbf{p}$ formalisms represent the back bone of semiconductor device modelling and were employed to study semiconductor nanostructures of a wide range of shapes, dimensions, and material compositions [2–4]. In the following, we discuss specific properties of semiconductor nanowires that need to be taken into account in the modelling process as well as the advantages and limitations of the above continuum models.

II. INFLUENCE OF THE FREE SIDE FACETS

The free side facets of nanowires represent steep barriers within the simulation of electronic properties. While barriers in quantum dots or planar layers are defined by the conduction and valence band offsets between the materials involved, the free side facets of nanowires represent a transition from the crystal to the vacuum. The main confining mechanism for the electron is thus the potential barrier resulting from the work function. The energy to create a hole in the valence band (i.e. the valence band barrier at the side facet) is the sum of the crystal's band gap and the electron affinity. As work functions and electron affinities are commonly large in comparison to band offsets between different alloys, the assumption of infinite barriers at the nanowire side facets is justified in most cases, in particular for the electrons and holes closest to the band gap [5]. An additional influence on the electronic properties of nanowires arises from surface potentials. Donors, that are either incorporated deliberately or unintentionally during the growth process, transfer extra electrons to surface states and thus remain ionized and the nanowire depleted. If the nanowire radius does not exceed the typical thickness of the depletion region of the bulk material, this feature gives rise to surface potentials that significantly alter the band profile throughout the whole nanowire [6].

Finally, dielectric confinement increases the potential experienced by charge carriers in nanowires due to the large difference between the dielectric constants inside and outside the nanowire, a feature which is of particular importance for thin nanowires [7].

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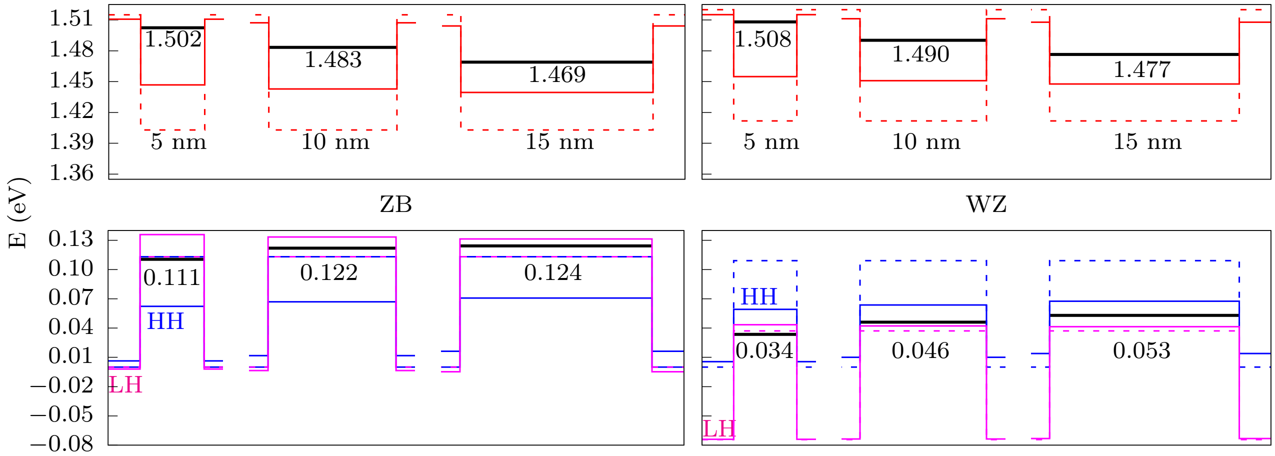

Fig. 1. Band offsets in (In,Ga)As/GaAs core-shell nanowire segments consisting of the zincblende (left) and the wurtzite phase (right) for an In content of 15% and (In,Ga)As shell thicknesses of 5, 10, and 15 nm. Dashed lines denote the band offsets without taking strain-induced modifications of the band profile into accound. Red lines indicate the conduction bands, blue and purple the heavy and light-hole bands, respectively. Energies of the electron and ground states are indicated using solid black lines with exact values below in eV.

III. SPECIFICS OF CRYSTAL-PHASE HETEROSTRUCTURES

Crystal-phase heterostructures consist of different crystal polytypes of chemically identical materials. Their main advantage over compositional heterostructures is that they exhibit atomically flat interfaces and induce only small elastic perturbations [8]. We illustrate the characteristic features of crystal-phase nanostructures for GaAs nanowires consisting of segments of both the zincblende and the wurtzite phase. First of all, a band offset between the conduction and valence bands of the respective phases occurs. The nature of this offset is usually of type II: the conduction band has its minimum in the zincblende phase, whereas the valence band maximum is located in the wurtzite phase. In wurtzite GaAs, an additional conduction band of Γ_8 character exists close to the Γ_7 conduction band such that both bands need to be taken into account in any model – a feature that is not contained in the eight-band $\mathbf{k} \cdot \mathbf{p}$ approach which to date represents the backbone of most device simulation tools. We note that this band is also present in wurtzite InAs, about 400 meV above the Γ_7 band. The energetical ordering of the Γ_7 and Γ_8 bands is influenced by strain: depending on the elastic properties of the system, either of the two conduction bands can dominate the confinement of electrons and their recombination process with holes [9,10]. A similar behavior is observed for the valence bands: while light and heavy holes are degenerate at the valence band maximum in the zincblende phase, the light hole band clearly dominates under the influence of strain while in the wurtzite phase the heavy hole dominates the character of the hole state.

IV. (IN,GA)AS/GAAS CORE-SHELL NANOWIRES

We have compared the electronic properties of (In,Ga)As/GaAs core-shell nanowires in the wurtzite and the zincblende phase in close collaboration with experiment. Our simulations have identified an energy difference between emission from otherwise identical zincblende and wurtzite segments that cannot be explained with the small band gap difference between the two polytypes. Instead, this energy difference results from the behavior of the valence band under the influence of strain inside the (In,Ga)As shell. While the light hole dominates the valence band under strain in the zincblende phase, the heavy-hole band becomes important in the wurtzite phase, due to crystal-field splitting. The band modifications and resulting electron and hole ground state energies can be seen in Fig. 1. Together with a reduced In content in the wurtzite phase, this effect can explain the observed discrepancy between luminescence peaks in the zincblende and the wurtzite phase.

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