Simulations of the electronic properties of GaAs polytype superlattices

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***Abstract*—We study the electronic properties of GaAs superlattices consisting of zincblende and wurtzite segments using a ten-band $\mathbf{k}\cdot\mathbf{p}$ model. Our simulations indicate that the simultaneous treatment of both the Γ_7 and the Γ_8 conduction bands is essential to achieve an accurate description of electron wave functions and energies.**

I. Introduction

GaAs can be considered as the prototype compound semiconductor material and is used for a wide range of applications from infrared light emission to acoustic sensoring, transistor technology and photovoltaic applications. In planar-layer growth, this material crystallizes in the cubic zincblende (ZB) phase, and the material properties of ZB GaAs have correspondingly been extensively studied and are well understood nowadays. Over the last decade, the growth and properties of semiconductor nanowires (NWs) have become a very active research field, leading to exciting discoveries and novel applications. A particularly important phenomenon is that many compound semiconductors, including GaAs, can crystallize during NW growth also in the metastable wurtzite (WZ) phase. A typical GaAs NW thus consists of a number of segments of WZ and ZB phases, which turns such a system into an axial *crystal-phase quantum structure* with complex electronic properties. The hexagonal phase of GaAs is difficult to produce in planar growth [1], so that the electronic properties of WZ GaAs remain poorly known. This makes NWs consisting of WZ and ZB segments the only structures available to approach the electronic properties of WZ GaAs from experiment. In recent years, much research interest has been dedicated to achieve a fundamental understanding of the properties of WZ GaAs [2-9] and many discrepancies were found between these studies. Most of the material parameters describing the electronic structure of WZ GaAs are still a matter of controversial discussion. In the present work, we evaluate existing parameter sets and introduce a ten-band $\mathbf{k}\cdot\mathbf{p}$ model that accounts for the specifics of the electronic structure of polytype GaAs NWs. We employ this model to compute the electronic structure of ZB/WZ superlattices (SLs) as well as GaAs NWs. Finally, we discuss the consequences of our findings for SLs and NWs.

II. Electronic properties of wurtzite GaAs

All of the previous studies on mixed-phase GaAs NWs report a type II band alignment between ZB and WZ segments,

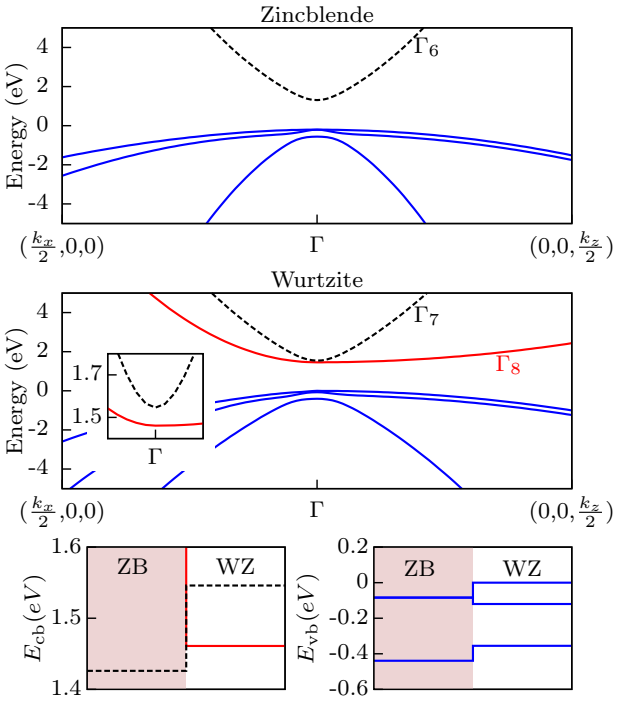

Fig. 1. Band structures of ZB (top) and WZ (center) GaAs using the parameters given in Ref. [7]. The VBs are depicted in blue, Γ_6, Γ_7 CBs are shown as dahed lines and the solid red line shows the Γ_8 CB. The inset shows a magnification of the two CBs around the Γ point in the WZ lattice. Bottom: CB (left) and VB (right) energy offsets between the two polytypes at the Γ point.

where the conduction band (CB) minimum is located in the ZB and the valence band (VB) maximum in the WZ segments. The band gap of WZ GaAs is reported to be larger than in the ZB phase in some studies [8,10] and smaller in others [2,7]. For the VB (CB) offsets, values of 55 (15) meV [10] to 117 (149) meV [8] have been reported. Of particular importance, however, is the dispersion relation of the CB in bulk WZ GaAs. For the ZB structure, the lowest CB is of Γ_6 character and well separated in energy from any remote CB [8]. In the WZ structure, the Γ_8 band results from zone folding due to doubling of the WZ unit cell along the [0001] direction in comparison to the ZB unit cell. In WZ GaAs, recent studies [2,5,7,8] indicate that the Γ_8 band is very close in energy to the Γ_7 band (which is the equivalent to the Γ_6 band in the ZB

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structure) (cf. Fig. 1). Moreover, it is unclear which of the two bands is lowest in energy: some studies find the Γ_7 band to be lower in energy than the Γ_8 band [8,11,12], others report the opposite [2,3,5,7]. Previous theoretical studies have employed only a single CB, where the difference between the characters of the bands was considered only via their different effective masses [2,13,14] or the strength of their dipole matrix element, thus treating them as one single hybrid band [15]. None of these studies considers the two bands separately.

Here we suggest a model based on a ten-band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian, that treats the Γ_7 and the Γ_8 band on equal footing. The Hamiltonian is an expansion of the eight-band model in Ref. [16], where the Γ_8 band has been added. While the treatment of the VBs at the ZB-WZ interface is more or less straightforward, the CBs form two intersecting potentials (cf. Fig. 1, bottom). As the Γ_8 band in the WZ results from zone folding of the L valley of the ZB phase, it has no equivalent in the ZB phase at the Γ point. We therefore assume the barrier height of this band to be given by the second lowest CB in the ZB phase, which is approximately 1.5 eV above the WZ Γ_8. Note that the assumption of an infinite barrier is also reasonable, given the large effective mass of the Γ_8 band. The coupling between the two CBs as well as between Γ_8 and the three VBs taken into account is assumed to be zero, so that the Γ_8 band is parabolic, but anisotropic. The ten-band model was implemented within the S/Phi/nx software library [17,18].

III. Zincblende/wurtzite superlattice

As a first step, we have computed the four lowest electron states of a planar ZB/WZ SL using our ten-band model and the parameters reported by De and Pryor [7]. The simplification of a planar system is justified here, as radial dependencies of strain and electrostatic potentials play only a negligible role in GaAs NWs. However, the spontaneous polarization within the WZ segment modifies the bulk band offsets and is taken into account. The energies of these states are shown in Fig. 2 as a function of the thickness of the two segments. The total size of the super cell along the [0001] direction is 40 nm. It is observed that the ground state as well as the two following excited states are of Γ_6 (Γ_7 in WZ) character for thin WZ segments, with their energy increasing with increasing thickness of the WZ segment. The character of the states changes to Γ_8 with increasing thickness (at 15 nm for the ground state, at 6 nm for the 1$^{\text{st}}$ and at 3 nm for the 2$^{\text{nd}}$ excited state). Due to the much larger effective mass of the Γ_8 band, the states are energetically closer in WZ-dominated SLs. Given that transitions from the VBs to the Γ_8 band are subject to a low oscillator strength [19], very long carrier lifetimes can be expected for these states if nonradiative recombination can be excluded such that recombination will be observed from much higher excited electron states that exhibit Γ_7 character. We emphasize that this behaviour depends crucially on the choice of the parameter set, in particular on the ordering of the two CBs. If the Γ_7 band is assumed to be lowest in energy, the electron ground state as well as the first excited states will be of Γ_7 character for all thicknesses of the two segments.

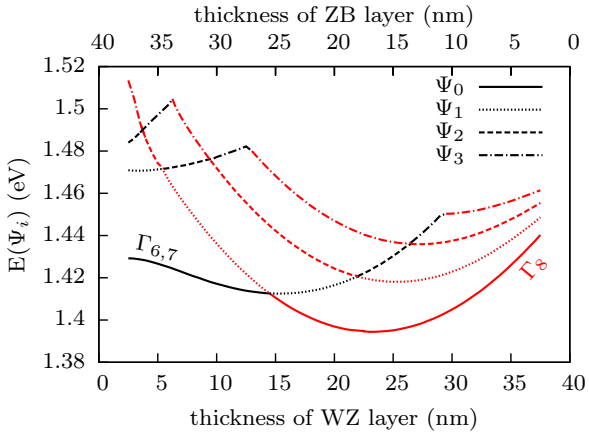

Fig. 2. Energies of the lowest electron states Ψ_i as a function of the thickness of WZ and ZB layer. Black lines indicate a Γ_6 or Γ_7 character, whereas red lines indicate that the character is Γ_8. The total size of the super cell along the [0001] direction is 40 nm. Energies refer to the WZ GaAs VB maximum.

However, even in this case (with a parameter set as the one provided in Ref. [8]), the Γ_8 band starts to dominate the electron states for thin GaAs NWs due to lateral confinement and the fact that the effective mass of this band is much larger than the one of the Γ_7 band.

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