Influence of random alloy fluctuations on the electronic properties of axial $In_xGa_{1-x}N$/GaN nanowire heterostructures

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***Abstract*—Compound semiconductor heterostructures such as quantum dots, nanowires, or thin films, are commonly subject to randomly fluctuating alloy compositions if they contain ternary and quaternary alloys. These effects are obviously of an atomistic nature and thus rarely considered in heterostructure designs that require simulations on a continuum level for theory-guided design or interpretation of observations. In the following, we present a systematic approach to the treatment of alloy fluctuations in (In,Ga)N/GaN thin films and axial nanowire heterostructures. We demonstrate to what extent random alloy fluctuations can be treated in a continuum picture and discuss the impact of alloy fluctuations on the electronic properties of planar and nano wire-based (In,Ga)N/GaN heterostructures.**

I. Introduction

Axial $In_xGa_{1-x}N$/GaN nanowire heterostructures represent a promising alternative to planar heterostructures for novel optoelectronic devices as their free side facets facilitate elastic relaxation even for large In contents of the active layer [1], [2]. The ternary alloy $In_xGa_{1-x}N$ acting as active layer furthermore facilitates light emission throughout the whole visible spectrum by controlling its In content x. On the other hand, a ternary alloy will inevitably exhibit local random alloy fluctuations (RAFs) throughout nanostructures spanning several 100 to a few 1000 nm^3. For (In,Ga)N alloys, it has been shown that the assumption of a homogeneous alloy is highly questionable [3], [4]. In the following, we provide a systematic study of the impact of RAFs in $In_xGa_{1-x}N$/GaN heterostructures on their optoelectronic properties using an eight-band $\mathbf{k}\cdot\mathbf{p}$ model that has been benchmarked against atomistic tight-binding calculations.

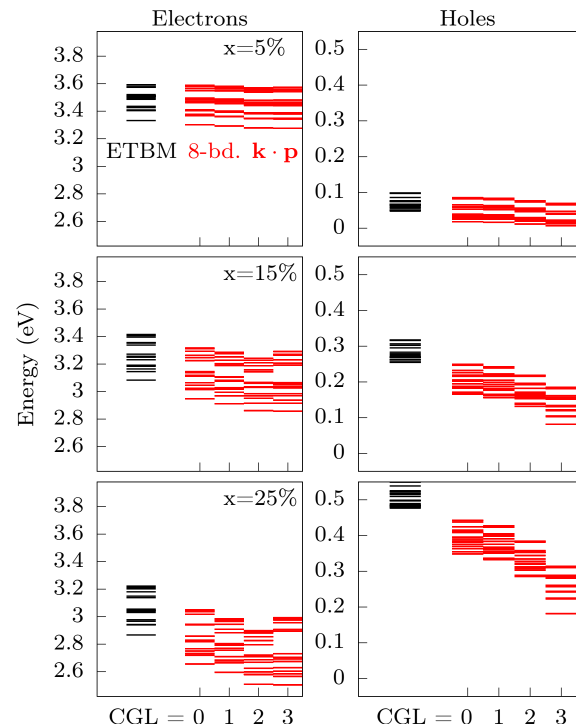

Fig. 1. Single-particle energies of the 15 electron (left) and hole (right) states closest to the band edges for different average In contents of an $In_xGa_{1-x}N$ layer with randomly fluctuating alloy composition in GaN. Black: computed using an atomistic empirical tight binding model. Red: computed using an eight-band $\mathbf{k}\cdot\mathbf{p}$ model for different coarse-graining levels (CGLs).

II. Comparison: atomistic and continuum model

We have systematically studied the capabilities of the continuum-based eight-band $\mathbf{k}\cdot\mathbf{p}$ formalism to account for

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RAFs and to investigate their impact on the electronic properties of (In,Ga)N/GaN heterostructures. In a first step, we have compared electron and hole energies in a planar $In_xGa_{1-x}N$ film of a thickness of 3 nm in GaN, that is subject to RAFs. For this purpose, we have set up randomized atomistic distributions of In atoms corresponding to average In contents of 5 – 25% inside the (In,Ga)N layer in an empirical tight-binding model. After computing the first 15 electron and hole states closest to the band edges, we have interpolated local average In contents for the cell of $10.2\times8.8\times7.8$ nm^3, discretized into $80\times80\times80$ (Coarse-graining level, CGL, 0) grid points. Using this – now continuum-based – representation, we have again computed the same electronic states using an eight-band $\mathbf{k}\cdot\mathbf{p}$ model [5] (cf. Fig. 1). We have employed the generalized multiband $\mathbf{k}\cdot\mathbf{p}$ module of the SPHInX library [6], [7], [8] and the respective material parameters can be found in Refs. [9] and [10]. It can be seen that – while individual states cannot always be resolved in terms of localisation and energy – there is an overall good agreement between the atomistic and the continuum model in terms of both ground state transition energy and spectral range of the 15 states computed. This agreement also holds to a good extent after coarse-graining the simulation cell to $40\times40\times40$ (CGL 1) and even $20\times20\times20$ (CGL 2), but is visibly reduced for a cell discretization of only $10\times10\times10$ grid points for the above simulation cell (CGL 3).

III. $In_xGa_{1-x}N$/GaN NANOWIRES

After estimating a grid discretisation of about 0.5 nm per direction as a reasonable compromise between accuracy and computational effort, we have performed a statistical analysis of the influence of RAFs on the electronic properties of GaN nanowires containing an axial $In_xGa_{1-x}N$ insertion. We have computed the electron and hole ground state charge density and transition energy and furthermore the exciton binding energy via a self-consistent Hartree approach [11]. Figure 2 shows the electron (red) and hole (blue) ground state density for the maximal and minimal exciton binding energy observed in 200 simulations with randomized In content inside the active layer for selected model nanowires (characteristic In content, layer thickness, and wire diameter given in the top row). We also show the corresponding properties of the respective reference system assuming a homogeneous alloy without any fluctuations inside the active layer as well as histograms of the exciton binding energies in the bottom row.

We find that RAFs induce variations of the exciton binding energy by a few tens of meV in otherwise identical nanowire heterostructures. For the thicker wires, alloy fluctuations can even double the exciton binding energy in some cases, as compared to a reference system with homogeneous In distribution, which we attribute to local clusters with large In content. The exciton binding energies show less variations for thin wires due to the fact that here the large potential barrier induced by the side facets enforces a more uniform confinement that is less sensitive to local fluctuations of the In content. However, there remains a nonnegligible impact of RAFs even in nanowires of only 10 nm diameter.

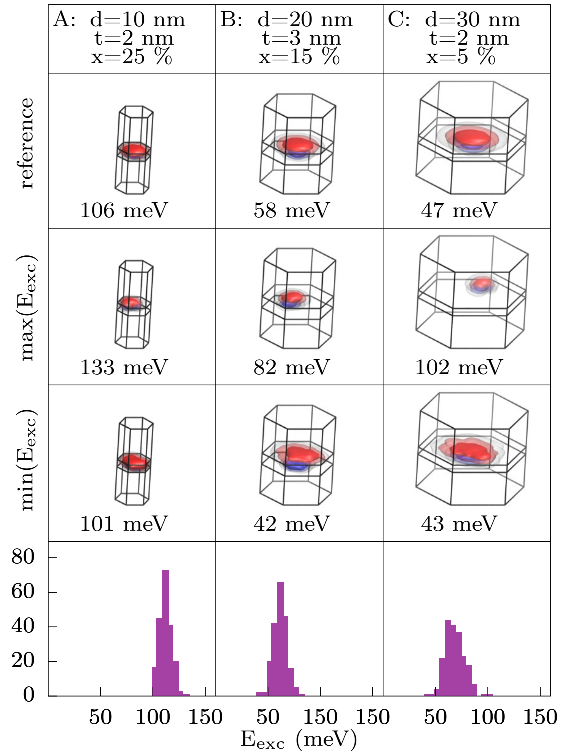

Fig. 2. Electron (red) and hole (blue) ground state charge density for the case of maximum and minimum exciton binding energy observed throughout 200 simulations with randomized, fluctuating In content in the active layer for three selected model systems, along with the reference data of the respective systems assuming a homogeneous alloy without any fluctuations. The corresponding exciton binding energies are provided as numbers and the bottom row shows the statistical distribution of exciton binding energies observed for each model system.

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