Impact of individual dopants on the electronic properties of axial $In_xGa_{1-x}N$/GaN nanowire heterostructures

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***Abstract*—We investigate the impact of individual ionized donors on the electronic properties of axial $In_xGa_{1-x}N$/GaN nanowire heterostructures. Our simulations indicate a strong impact of the electrostatic potential arising from ionized donors on the charge carrier confinement. A statistical analysis of nanowires containing randomly distributed donors reveals a large wire-to-wire variation of transition energies and electron-hole overlap, which contributes to a broadening of the emission lines in ensembles of axial $In_xGa_{1-x}N$/GaN nanowire heterostructures. Additionally, we systematically study the influence of a single donor in the vicinity of the active $In_xGa_{1-x}N$ layer and discuss the impact of the donor for different In contents x.**

I. Introduction

The conductivity of semiconductors can be tuned over many orders of magnitude by the intentional incorporation of impurities [1]. All semiconductor-based technology therefore depends on the ability to dope the material in a controlled fashion [2], [3]. For the theoretical description of semiconductor devices, doping represents a formidable problem, since dopants occupy random positions at the host lattice, such that established solid-state methods exploiting the periodicity of the crystal cannot be employed [4]. The discrete nature of randomly distributed dopants is commonly ignored in device simulation models, and a homogeneous, continuous distribution of charge is assumed [5]. With modern electronic devices approaching dimensions of a few tens of nm, however, their core semiconductor structures contain a countable number of dopants and charge carriers are thus strongly influenced by a complex potential landscape arising from the randomly distributed dopants. The large fluctuations of both number and position of the dopants may therefore dominate the electronic properties of the device [5].

We have recently discussed the influence of surface potentials arising from unintentional doping and Fermi level pinning on the electronic properties of axial $In_xGa_{1-x}N$/GaN nanowire (NW) heterostructures and identified a nontrivial interplay of surface and polarization potentials [6]. While this study provided a qualitative explanation for the experimentally observed reduction of photoluminescence (PL) intensity for low In contents or thin $In_xGa_{1-x}N$ layers, we have assumed a homogeneous charge density arising from unintentional n-type doping here. The maximum doping density considered in our previous study was 10^{17} cm^{-3}, which corresponds to an average of 8.3 charges in a hexagonal NW segment of 20 nm length and 80 nm diameter, such that a more realistic picture needs to consider randomly distributed donors rather than a homogeneous doping-related charge density. The present work is a statistical study of the influence of random dopant fluctuations (RDF) on electron and hole localization and energies.

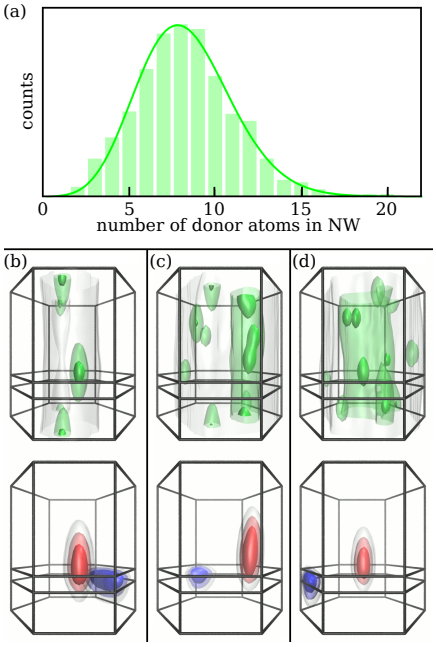

Fig. 1. (a) statistical distribution of the number of donors in the NW. (b)-(d): Electrostatic potential (top) and electron (red) and hole (blue) ground state charge density (bottom) for NWs containing 3 (b), 9 (c) and 13 (d) donors (not to scale).

II. Electronic structure of $In_xGa_{1-x}N$/GaN NWs containing randomly distributed donors

Si and O represent the typical unintentionally incorporated donors in $In_xGa_{1-x}N$/GaN NWs. With doping densities of about 10^{17} cm^{-3}, both these atoms induce only negligible elastic deformations of the host lattice [7]. They can furthermore be considered as shallow donors, and we assume that all donors transfer their extra electron to surface states on the NW

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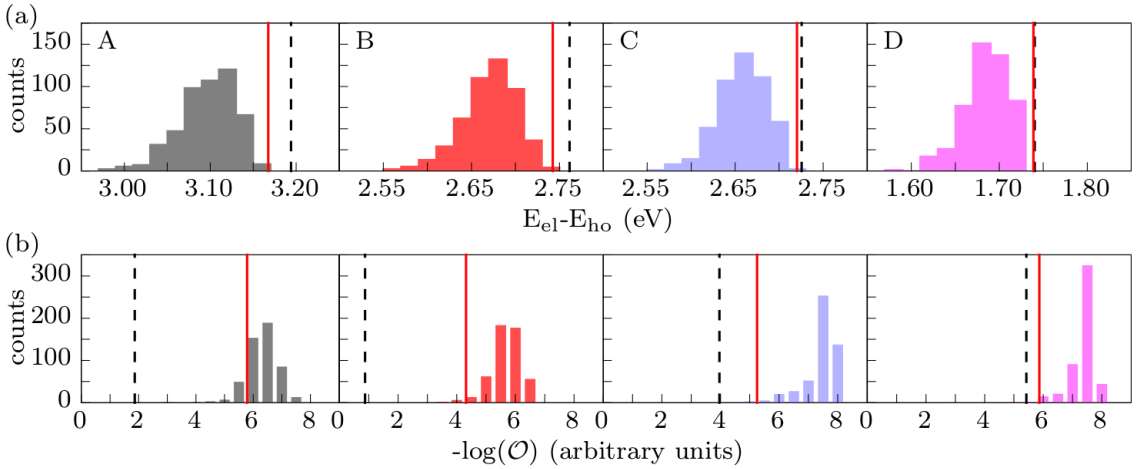

Fig. 2. (a) Histograms of the ground state transition energy, E_{el}-E_{ho}, for the four configurations. Red solid and black dashed lines indicate the cases of a homogeneous doping charge and of an undoped NW, respectively. (b): Histograms of the electron-hole overlap $\mathcal{O}$. Note the negative logarithmic x-axis.

side facets. In this case, we can model randomly distributed donors in a NW simply as point charges with a Coulomb potential. In the next step, this Coulomb potential enters an eight-band $\mathbf{k} \cdot \mathbf{p}$ model as an additional potential contribution to compute electron and hole wave functions and energies.

The system under consideration is a hexagonal GaN NW of a diameter of 80 nm with an $In_xGa_{1-x}N$ disk of thickness t. We have studied four different configurations of In content and disk thickness: two thin layers (t=1 nm) with 5% (A) and 30% (B) In content and two thick layers (t=5 nm) of 10% (C) and 30% (D) In content. We have then performed a statistical study of 500 different random distributions of donors corresponding in average to a doping density of 10^{17} cm^{-3} for each of our four model configurations.

Figure 1 shows the statistical distribution of the number of donors (a) as well as three examplary electrostatic potentials resulting from doping together with the respective electron and hole ground state charge densities (b)-(d) in a side view of the NW. Both charge carriers are confined in the vicinity of the active layer with the electron on the top and the hole on the bottom facet due to the piezoelectric potential. However, it can be seen that the confinement of both charge carriers is strongly influenced by the presence of donors. In particular, the electron confinement is governed by the attractive Coulomb potential of the donors.

The histograms of the ground state recombination energy are shown in Fig. 2. For all four configurations, we observe energy variations of approximately 100 meV. This indicates that even if fluctuations of the In content or the thickness of the active layer or variations of the NW diameter could be excluded, a significant broadening of emission lines will be observed originating solely from RDFs. The recombination energy obtained when assuming a homogeneous doping charge density, as used in Ref. [6], is indicated as a solid red line. Additionally, the case of an ideal, doping-free NW is indicated with a black dashed line. The energies for the case of randomly distributed individual donors is always smaller than for these two cases. This finding results from the fact that individual donors induce deeper potential wells, in contrast to a homogeneous charge density, thus lowering the energy of the electrons localized in the vicinity of the donors.

The electron-hole ground state overlap $\mathcal{O}$ as defined in Ref. [6] is shown in Fig. 2 (b), and is seen to vary by four orders of magnitude. The overlap is furthermore smaller than the one for the assumption of a homogeneous doping charge as the donor-induced potentials lead to strong localization of the electrons whereas the hole is localized mainly due to the polarization potential of the active layer. For all four cases, the ideal, doping-free NW represents an upper limit of both the overlap as well as the ground state transition energy (dashed black line in Fig. 2.)

In conclusion, we have shown that RDFs have a severe influence on the electronic properties of $In_xGa_{1-x}N$/GaN NW heterostructures, leading to a broadening of the ensemble emission lines even in otherwise identical NWs and a significant reduction of the electron-hole overlap. RDFs represent a fundamental obstacle for devices that rely on well-defined energy levels. In single-photon emitters based on III-nitride NWs, the presence of individual dopants in a NW will modify the electronic structure and thus make it difficult to obtain reproducible wavelengths. NW-based devices for the generation of entangled photons will also suffer from RDFs, which will reduce the overall symmetry of the system.

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