

Minimizing the influence of surface potentials in axial $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ nanowire heterostructures by reducing their diameter

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Abstract—Simulations using continuum elasticity theory and an eight-band $k\cdot p$ approach suggest the reduction of the diameter of $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ axial nanowire heterostructures to be a promising approach to increase the intensity of light emitting processes. A reduction of the nanowire diameter significantly reduces the magnitude of surface potentials and thus leads to a much larger overlap of the electron and hole charge densities.

I. INTRODUCTION

The ternary alloy $\text{In}_x\text{Ga}_{1-x}\text{N}$ appears to be a highly promising candidate for the development of phosphor-free white light-emitting diodes (LEDs), as its band gap covers the whole visible spectrum [1], [2]. However, the large lattice mismatch between GaN and InN and the tendency of phase separation make it difficult to synthesize planar $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ quantum well structures with high In contents and a high structural perfection. The internal quantum efficiency (IQE) of conventional, planar $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based LEDs therefore drops with increasing emission wavelength.

GaN nanowires (NWs) with axial $\text{In}_x\text{Ga}_{1-x}\text{N}$ insertions represent an attractive alternative to planar $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures, as the elastic strain resulting from the lattice mismatch between $\text{In}_x\text{Ga}_{1-x}\text{N}$ and GaN can at least partly be relieved elastically at the free side facets. The elastic relaxation moreover leads to reduced piezoelectric fields, which is expected to improve the electron-hole overlap and thus to increase the internal quantum efficiency (IQE) [3]. In fact, axial $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ NW heterostructures have been reported to emit in the green, amber and red range of the visible spectrum [4], [5], [6]. On the other hand, it was observed that the photoluminescence (PL) intensity of such structures decreases with decreasing In content, and it was found to be difficult to obtain light emission in the blue or violet spectral range [7]—a behavior which is exactly the opposite of what is commonly observed in planar heterostructures.

We have previously identified surface potentials resulting from Fermi level pinning and residual doping as a likely origin of this counterintuitive behavior [8]. In our previous work, we have calculated the electron and hole states confined in an $\text{In}_x\text{Ga}_{1-x}\text{N}$ quantum disk inserted in a GaN NW for a wide range of In contents and disk thicknesses and could qualitatively reproduce the experimentally observed behaviour. The diameter of the NWs that were studied in Ref. [8] was

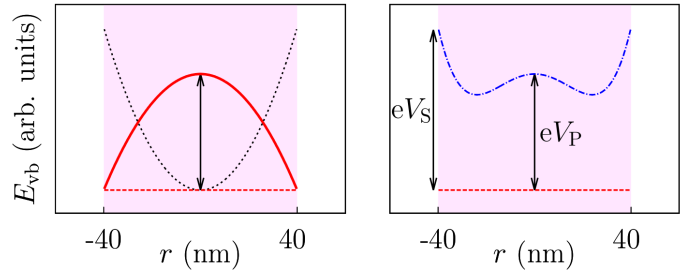


Fig. 1. (Color online) Left: qualitative valence band edge modification due to polarization (solid red) and surface potential (dotted black) at the bottom of the $\text{In}_x\text{Ga}_{1-x}\text{N}$ disk. Right: combination of both potentials.

kept constant. In a recent study on lithographically etched $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ NWs, a significant improvement of the IQE has been reported when reducing the NW diameter [9]. We have thus extended our previous work to a systematic investigation of the influence of the NW diameter on the confinement of electrons and holes in the $\text{In}_x\text{Ga}_{1-x}\text{N}$ quantum disk. We suggest that a reduction of the diameter below 40 nm—a range which is still experimentally accessible—leads to a significant increase of the IQE.

II. INTERPLAY OF SURFACE AND POLARIZATION POTENTIALS

The confinement of electrons and holes in axial $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ nanowire heterostructures is governed by three different mechanisms. First of all, *conduction- and valence band offsets* induce a confinement of both electrons and holes within the center of the $\text{In}_x\text{Ga}_{1-x}\text{N}$ disk. As a second effect, a *polarization potential* forms throughout the disk and the surrounding material, leading to a spatial separation of electrons and holes along the growth direction (the [0001]-direction)—a behaviour which is well understood for planar structures. In axial NW heterostructures, the extrema of this potential are in the center of its top and bottom interfaces due to the three-dimensional nature of the $\text{In}_x\text{Ga}_{1-x}\text{N}$ insertion and the associated inhomogeneous strain relaxation [10]. The third charge confining mechanism in semiconductor NWs is the *surface potential*, which arises from Fermi level pinning and residual doping. For n-type GaN, the surfaces represent

an attractive potential for hole states. While the electron states are confined along the central axis of the NW due to both the surface and the three-dimensional polarization potential, the hole state confinement is dominated by either the polarization or the surface potential (cf. Fig 1) [8].

The reduction of the PL intensity for smaller wavelengths can now be understood as a consequence of an interplay between surface and polarization potentials. Small wavelengths are associated with thin $\text{In}_x\text{Ga}_{1-x}\text{N}$ disks or small In contents, where the corresponding polarization potentials are weak and the hole state localization is governed by the surface potentials, which leads to an in-plane spatial separation of electrons and holes. Longer wavelengths require higher In contents or thicker disks, which induce strong polarization potentials that dominate the hole state localization. Thus, both electrons and holes are localized along the central axis of the NW, and spatially separated only along the growth direction. Given that the diameter of the NWs is one order of magnitude larger than the thickness of the $\text{In}_x\text{Ga}_{1-x}\text{N}$ -disk, the electron-hole overlap is much larger in the latter case (cf. Fig. 2).

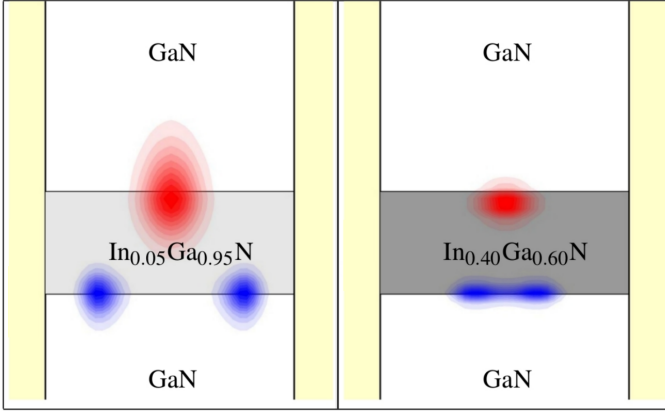


Fig. 2. Electron (red) and hole (blue) ground state charge densities for low (left) and high (right) In content x . White and grey areas depict the nanowire and the $\text{In}_x\text{Ga}_{1-x}\text{N}$ disk, respectively. Here, a doping density of $N_D = 5 \times 10^{16} \text{ cm}^{-3}$, a disk thickness of 5 nm and a NW diameter of 80 nm were assumed. Note that the plot is not to scale.

III. RESULTS AND DISCUSSION

Assuming a homogeneous density of doping charges, the surface potential depends quadratically on the NW diameter. It can therefore be expected that a reduced diameter leads to a significant reduction of the in-plane spatial separation of electrons and holes [11]. We have computed the electron and hole ground state charge densities for different system configurations as a function of the NW diameter. The configurations considered are (A) a thick $\text{In}_x\text{Ga}_{1-x}\text{N}$ disk of 5 nm thickness and $x=10\%$, and two disks with each 1 nm thickness and $x=30\%$ (B) and $x=5\%$ (C). As a measure for the spatial separation of electrons and holes, we use the charge carrier overlap \mathcal{O} , as defined in Ref. [8]. Figure 3 shows \mathcal{O} for the three model configurations as a function of the NW diameter d for different doping densities N_D . In all three plots,

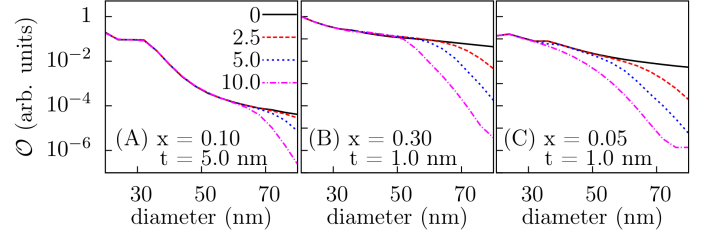


Fig. 3. Electron-hole ground state overlap \mathcal{O} as a function of the NW diameter d for different doping densities N_D for the configurations A (left), B (middle) and C (right). The doping densities corresponding to each curve are given in the left plot in units of 10^{16} cm^{-3} . Discontinuities in the plots of configuration A and C result from a switching of the hole ground state between s- and p-like character.

the electron-hole overlap is not visibly influenced by doping below a certain diameter. Even in configuration (C), where the surface potentials tend to dominate the hole state confinement, their influence is small when reducing d to 40 nm or less. For larger diameters, surface potentials arising from larger doping levels lead to a reduction of the electron-hole overlap by orders of magnitude. In case (A), where surface potentials play a less pronounced role compared to the polarization due to the large disk thickness, the overlap is reduced by two orders of magnitude. In cases (B) and (C), the surface potentials lead to a reduction of the overlap of four orders of magnitude for a NW diameter of 80 nm.

Our simulations reveal a significant impact of the NW diameter on the surface potential and thus on the spatial separation of electrons and holes. For diameters below 40 nm, the influence of surface potentials is almost negligible, whereas it becomes the dominant potential for hole state confinement for larger diameters, leading to a complete in-plane spatial separation of electrons and holes. We therefore conclude that reducing the diameter of axial $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ NWs below 40 nm can lead to a significant improvement of the efficiency of NW-based LEDs.

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