Influence of surface and polarization potentials on the electronic and optical properties of $In_xGa_{1-x}N$/GaN axial nanowire heterostructures

Oliver Marquardt, Christian Hauswald, Martin Wölz, Lutz Geelhaar, and Oliver Brandt
Paul-Drude-Institut für Festkörperelektronik
Hausvogteiplatz 5–7, 10117 Berlin, Germany
Email: marquardt@pdi-berlin.de

***Abstract*—We study the influence of surface and polarization potentials on the electronic properties of axial $In_xGa_{1-x}N$/GaN nanowire heterostructures. Our simulations indicate nontrivial, competing influences of both these potentials on the spatial separation of electrons and holes, which are well suited to explain previous experimental observations.**

I. Introduction

$In_xGa_{1-x}N$ is considered to be an excellent, environmentally friendly canditate for novel light emitting devices spanning the whole visible spectrum [1], [2]. The growth of planar $In_xGa_{1-x}N$/GaN nanostructures, however, is limited by the large lattice mismatch between GaN and InN and the tendency of phase separation. Hence, the crystal quality required for light emitting devices cannot be achieved throughout the whole composition range. This drawback of planar $In_xGa_{1-x}N$/GaN heterostructures can in principle be avoided in $In_xGa_{1-x}N$/GaN axial nanowire heterostructures. Here, an $In_xGa_{1-x}N$ disk serves as the active region for light emission in a GaN nanowire. The nanowire geometry facilitates elastic relaxation of the strained disk due to the free surfaces even for large In contents. In fact, many studies report green, amber, and red light emission from axial $In_xGa_{1-x}N$/GaN heterostructures [3], [4], [5]. However, it was recently observed that the photoluminescence intensity monotonically decreases with decreasing In content, thus making light emission in the blue spectral range difficult to achieve [6]. In this paper, we report on a systematic study of the influence of the In content and the thickness of the active layer on the electronic properties of axial $In_xGa_{1-x}N$/GaN nanowire heterostructures. The simulation is based on continuum elasticity theory and an eight-band $\mathbf{k}\cdot\mathbf{p}$ model implemented within a plane-wave framework [7], [8], and takes strain, piezoelectricity, and surface potentials into account.

II. The role of piezoelectric polarization and surface potentials

Free surfaces allow for elastic relaxation of nanowires, thus reducing the strain, but also the piezoelectric polarization in and around the active region. Nevertheless, strain and piezoelectricity cannot be fully eliminated in nanowires and still influence the electronic properties of the system. In particular, polarization potentials V_P will occur that induce a spatial separation of electrons and holes along the growth direction, as is well-known and understood for planar III-nitride heterostructures. Due to the existence of free surfaces, nanowires furthermore exhibit surface potentials V_S resulting from Fermi level pinning and unintentional doping. These additional potentials represent an attractive potential for either hole or electron states and can therefore induce an in-plane spatial separation of the charge carriers. The influence of surface and polarization potentials on the valence band energy E_vb is depicted schematically in Fig. 1. Correspondingly, the charge carrier confinement and the resulting recombination rate will depend on the interplay between polarization potentials and surface potentials.

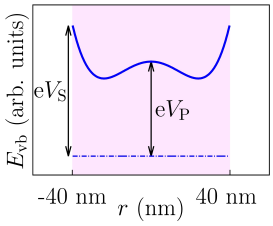

Fig. 1. Schematic line scan of the valence band edge at the bottom interface of an $In_xGa_{1-x}N$ insertion in a GaN nanowire along the wire's diameter, including surface potentials (eV_S) and polarization potentials (eV_P). The dashed line indicates the bulk valence band edge. The shaded area depicts the wire diameter.

As a first step towards understanding this interplay, we have considered a surface potential which decays quadratically towards the central axis of the nanowire. Assuming a Fermi level pinning of 0.6 eV above the conduction band edge [9] and a diameter of the nanowire of 80 nm, a doping level of $10^{17}\mathrm{cm}^{-3}$ corresponds to a surface potential drop of $eV_\mathrm{S} = 80$ meV. In order to achieve a qualitatively meaningful description of the influence of surface and polarization potentials on the charge carrier confinement, we have limited our study to the electron and hole ground states and used the spatial charge carrier overlap $\mathcal{O}$ as an indicator:

$$\mathcal{O} = \sum_{r_1}\sum_{r_2}\sum_{r_3} \varrho_\mathrm{e}(r_1,r_2,r_3)\varrho_\mathrm{h}(r_1,r_2,r_3) \qquad (1)$$

where r_i denotes the spatial discretization of the super cell and $\varrho_{e,h}$ represents the electron and hole charge densities.

978-1-4673-6310-5/13/$31.00 ©2013 IEEE

III. Results and Discussion

Our studies indicate that surface potentials dominate the hole state confinement for small In contents x, but also for small thicknesses t of the active layer, with the hole state confined close to the surfaces of the nanowire [Fig. 2, left]. In fact, we have experimentally observed this dependence on both the In content and the layer thickness in a recent study [10]. For larger In contents or layer thicknesses, the strength of the polarization potential increases, and the hole state charge density moves closer to the central axis of the nanowire. As the wire diameter is much larger than the thickness of the active layer, this results in an increase of the electron-hole overlap [Fig. 2, right]. A systematic plot of the overlap $\mathcal{O}$ for

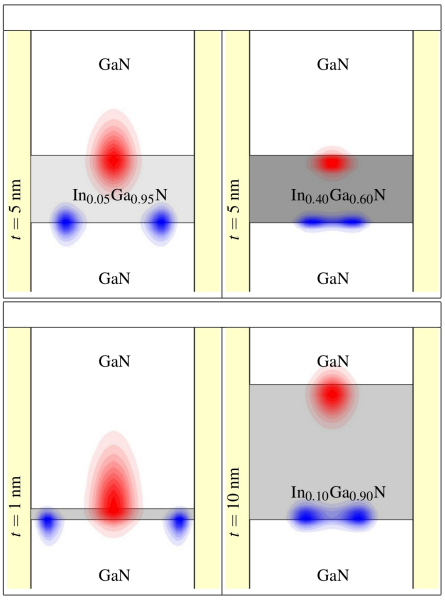

Fig. 2. Electron (red) and hole (blue) ground state charge densities for low (left) and high (right) In content x (top) and disk thickness t (bottom). White and grey areas depict the nanowire and the $In_xGa_{1-x}N$ disk, respectively. Here, the surface potential has a magnitude of 40 meV.

different surface potentials is shown in Fig. 3 as a function of the In content x [Fig. 3 (a)] and the layer thickness t [Fig. 3 (b)]. Surface potentials significantly reduce the charge carrier overlap, in particular for low In content and thin layers. The spatial separation of electrons and holes along the growth direction due to polarization is a well-known effect in polar III-nitride quantum wells: Increasing the In content or the layer thickness leads to a reduction of the internal quantum efficiency, whereas the opposite is the case in axial nanowire heterostructures due to the influence of surface potentials. In fact, the polarization potential with its extrema at the center of the top and bottom interface of the active layer is *required* to reduce the in-plane spatial separation of electrons and holes caused by the surface potential. To separate the in-plane spatial separation due to surface potentials from the one arising along the growth direction, we normalize the overlap by a one-dimensional projection of the overlap on the central axis of the wire, $\mathcal{O}_{1D}$. We can then visualize the data from Figs. 3 (a) and

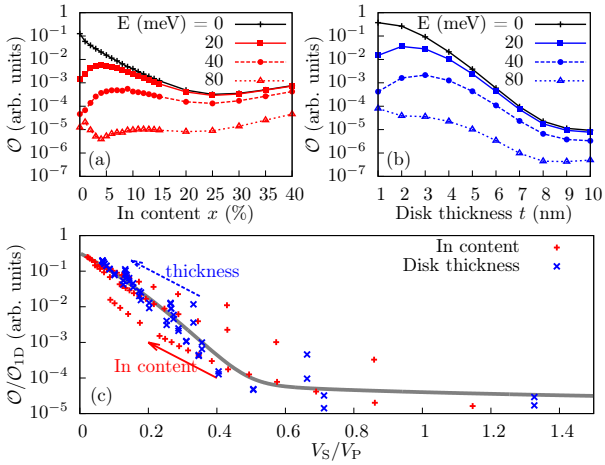

Fig. 3. Electron-hole ground state overlap $\mathcal{O}$ for different surface potentials as a function of the In content x (a) and of the disk thickness t (b). The bottom figure (c) shows a general trend of the normalized electron-hole overlap $\mathcal{O}/\mathcal{O}_{1D}$ including the data from the above plots as a function of the ratio between surface and polarization potential maxima. The grey line is a guide to the eye.

3 (b) as a function of the ratio between surface and polarization potentials $|V_S/V_P|$, enabling us to identify a general trend of the charge carrier overlap for different strengths of surface and polarization potentials as shown in Fig. 3 (c). In fact, we can see that the normalized overlap $\mathcal{O}/\mathcal{O}_{1D}$ decreases dramatically once the surface potentials dominate the charge carrier confinement.

We conclude that the elastic relaxation possible in nanowires, while enabling a higher In content in the active region, is in a certain sense counterproductive. The strain reduction and the resulting reduction of polarization fields lead to a reduced electron-hole overlap as the piezoelectric polarization is essential to compensate the in-plane separation of electrons and holes caused by surface potentials. To increase the light emission efficiency of such nanowire structures, it is of higher priority to reduce the surface potentials by passivating the surfaces or minimizing unintentional doping [10].

References

[1] S. Nakamura and G. Fasol, *The Blue Laser Diode* (Springer, Berlin, 1997).
[2] P. Rinke, M. Winkelnkemper, A. Qteish, D. Bimberg, J. Neugebauer, and M. Scheffler, Phys. Rev. B **77**, 075202 (2008).
[3] A. Kikuchi, M. Tada, K. Miwa, and K. Kishino, Proc. SPIE **6129**, 612905 (2006).
[4] R. Armitage and K. Tsubaki, Nanotech. **21**, 195202 (2010).
[5] W. Guo, M. Zhang, A. Banerjee, and P. Bhattacharya, Nano Lett. **10**, 3355 (2010).
[6] M. Wölz, J. Lähnemann, O. Brandt, V. M. Kaganer, M. Ramsteiner, C. Pfüller, C. Hauswald, C. N. Huang, L. Geelhaar, and H. Riechert, Nanotech. **23**, 455203 (2012).
[7] O. Marquardt, S. Boeck, C. Freysoldt, T. Hickel and J. Neugebauer, Computer Phys. Commun. **181**, 765 (2010).
[8] O. Marquardt, S. Schulz, C. Freysoldt, S. Boeck, T. Hickel, E. P. O'Reilly, and J. Neugebauer, Opt. Quant. Elec. **44**, 183 (2012).
[9] R. Calarco, M. Marso, T. Richter, A. Aykanat, R. Meijers, A. D. Hart, T. Stoica, and H. Lüth, Nano Lett. **5**, 981 (2005).
[10] O. Marquardt, C. Hauswald, M. Wölz, L. Geelhaar, and O. Brandt, (submitted to Nano Lett.).