

# Cubic $AlGaN/GaN$ and $GaN/InGaN$ heterostructures: effects of p-type doping

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Recently, increasing interest has been observed in group-III nitride semiconductor heterostructures, such as  $AlGaN/GaN$  and  $GaN/InGaN$  quantum wells (QWs) due to their important applications in high-power microelectronic and blue-green-UV optoelectronic devices as well as in modulation-doped field effect transistors. Although most of the progress achieved so far is based on the hexagonal (wurtzite)  $III-N$  materials, the cubic (c) metastable-phase layers are believed to possess potential advantages arising as promising alternatives for similar applications. Controlled p-type doping of GaN, AlGaN, and InGaN layers are of crucial importance in particular for some electronic and optoelectronic devices. However, this has been difficulted by the deep nature of the Mg acceptor. Several attempts have been made trying to enhance the acceptor doping efficiency, for example by using multiple QWs and superlattices (SLs) of alternate layers of GaN and AlGaN or InGaN. In wurtzite structures, these techniques have shown to lower the acceptor ionization energy, increasing the p-type conductivity by several orders of magnitude [1, 2]. This also provided evidence for the formation of a two-dimensional hole gas (2DHG) in the well regions of the heterostructures, which is induced by piezoelectric (PZ) and spontaneous polarization effects. Contrary to hexagonal materials, in p-doped cubic structures a 2DHG may arise, even in the absence of PZ fields, provided adequate design parameters for the heterostructures are employed.

In this work we investigate the effects of p-type doping and of the 2DHG present in  $Al_xGa_{1-x}N/GaN$  and  $GaN/In_xGa_{1-x}N$  multiple QWs and SLs in the c-phase, by carrying out self-consistent band structure calculations within a multiband (6 x 6) Luttinger-Kohn (LK) model in which the heavy, light, and spin-orbit split-off hole bands are included and in a plane-wave representation [3]. Firstly, the method recently developed by us [4] is extended to allow for self-consistency. Thus, the (6 x 6) LK effective mass equations are solved together with the Poisson equation for the charge distribution in the heterostructure. The different effective-mass parameters of well and barrier regions are properly taken into account. A supercell model approach which comprises the QW and the barrier is adopted; therefore, for large barrier widths the limit of isolated QWs is obtained. Secondly, the generalized method presented here is applied for a series of heterostructures in which well- and barrier-widths, alloy content, and acceptor doping concentration as well its profile are varied. Exchange-correlation effects within the 2DHG, taken into account in the local density approximation, are found to amount for about 10% of the total potential. Strain effects due to lattice mismatch, and their influence on the hole sub-bands and potential profiles are analyzed. Figs. 1 and 2 show the self-consistent hole sub-bands and potential profiles obtained for 60 Å centered barrier doped p-type  $AlGaN/GaN$  and  $GaN/InGaN$  SLs, respectively, for which equal acceptor doping concentration  $5 \times 10^{18} cm^{-3}$ , well-width of 100 Å and barrier width of 200 Å were considered. A valence-band offset of 40% was used in both systems. As expected, strain effects

are found to be stronger in InGaN-derived structures than in the AlGaN ones, due to the larger lattice mismatch for the formers. We show that for acceptor concentrations as high as  $10^{19} \text{cm}^{-3}$  the light-hole band may be occupied in AlGaN/GaN SLs.

The results shown here constitute the first attempt to investigate the limit conditions for the formation of a 2DHG and its physical features in cubic group-III nitride heterostructures. Their implications in the c-based optoelectronic devices are discussed.

## REFERENCES

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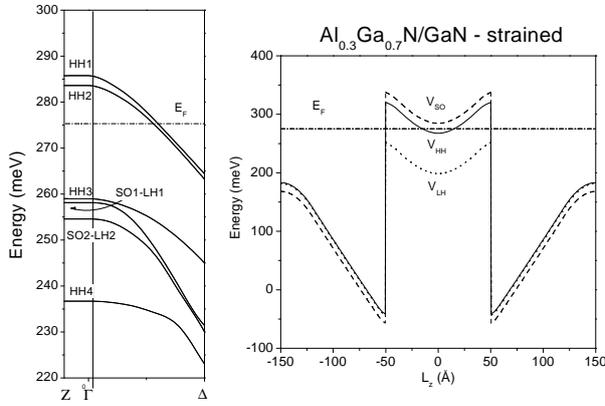


FIG. 1: Barrier-doped strained AlGaN/GaN SL: (left) hole sub-bands along SL symmetry lines  $\Gamma Z$  (growth-axis) and  $\Delta$  (perpendicular to growth-axis); (right) heavy, light, and split-off hole potential profiles. The Fermi level is indicated by  $E_F$ .

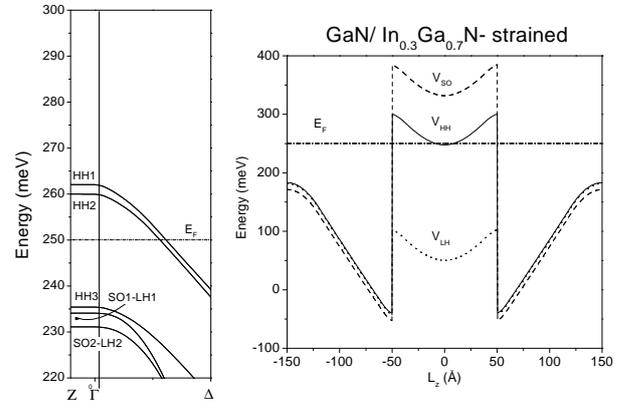


FIG. 2: Same as in Fig.1 for a barrier-doped strained GaN/InGaN SL.