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Polarization induced 2D hole gas in GaN/AlGaN heterostructures

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Abstract

The generation of high density 2D hole gases is crucial for further progress in the electronic and optoelectronic nitride devices. In this paper, we present systematic theoretical studies of Mg-doped GaN/AlGaN gated heterostructures and superlattices. Our calculations are based on a self-consistent solution of the multiband *k.p* Schrödinger and Poisson equation and reveal that the hole 2D sheet density is mainly determined by the polarization induced interface charges. For an aluminium concentration of 30%, the induced hole density in the heterostructure can reach values up to $1.5 \times 10^{13} \text{ cm}^{-2}$. In the GaN/AlGaN superlattices, the hole sheet density increases with the superlattice period and saturates for a period of 40 nm at a value of $1.5 \times 10^{13} \text{ cm}^{-2}$. © 2001 Elsevier Science B.V. All rights reserved.

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High concentrations of holes in GaN and AlGaN layers are required for the development of various electronic and optoelectronic nitride-based devices. The development of heterostructure bipolar transistors or laser diodes in the UV regime has been hampered by the high ionization energy of the Mg acceptor commonly used for p-type doping in nitrides. Recently, it has been reported that the low doping efficiency of the deep Mg acceptor can be overcome in nitride heterostructures by utilizing the strong pyro- and piezoelectric character of these materials [1–5].

Unstrained nitride layers exhibit spontaneous polarization, whereas in strained layers both spontaneous and piezoelectric polarization are present. The differences of the polarizations in the adjacent layers induce interface charges. These, in turn, cause strong internal electric fields that can pull the acceptor energies below the Fermi level. In this paper, we report extensive theoretical studies of the electronic structure of holes associated with the degenerate valence band and confined within GaN/AlGaN quantum wells and superlattices. Our calculations clearly show that the density of the two-dimensional hole gas (2DHG) is mainly controlled by the polarization charge at the GaN/AlGaN interface. Other factors, such as the widths of barriers and wells, the temperature, and the Mg-concentration profile play a minor role.

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Our calculations are based on the self-consistent multiband $k.p$ envelope function theory for holes [6]. The interaction of carriers with one another and with ionized acceptors has been treated within the Hartree approximation. Polarization induced surface charges at the interfaces have been included in the Poisson equation for the electrostatic potential. The system of 6×6 equations for the components of the envelope functions and the Poisson equation have been discretized on a non-uniform mesh. The dependence of the eigenstates on the lateral wave vector has been taken into account. The hole density has been calculated by summing over the discrete eigenstates, weighted by the Fermi distribution function, and by integrating over the lateral Brillouin zone. To the best of our knowledge, all previous reports were based on one band hole models and assumed a parabolic lateral dispersion [1,2,4,5].

The parameters of the 6×6 $k.p$ Hamiltonian matrix (including the 4 deformation potentials) for wurtzite GaN and AlN have been taken from ab initio calculations [7] and were linearly interpolated for AlGaIn alloys. The transverse interface charge that enters the Poisson equation has been determined as the difference in the normal components of the transverse polarization in adjacent materials. The values of the spontaneous polarization and piezoelectric constants have been taken from first-principle calculations for GaN and AlN [8] and we have linearly interpolated them for alloys. The strain in the materials has been calculated within elasticity theory. For this purpose, the interpolated experimental lattice and elastic constants of the constituent bulks [9] have been used.

First, we present results of our calculations for gated GaN/AlGaIn heterostructures consisting of a GaN substrate layer, a (0001)-pseudomorphically grown AlGaIn barrier, and a Schottky contact on top of it. To enhance the hole confinement on the GaN/AlGaIn interface through the negative polarization charge, the polarity of the sample must be of N-face type, i.e., the spontaneous polarization should point outwards from the substrate. For the GaN layer, we have assumed a homogeneous Mg-concentration of $1.6 \times 10^{17} \text{ cm}^{-3}$. The adjacent AlGaIn

barrier consists of a 5 nm undoped spacer and a homogeneously Mg-doped ($[\text{Mg}] = 5 \times 10^{19} \text{ cm}^{-3}$) layer. In our calculations, we have varied the barrier width from 15 to 35 nm and the Al content from 0% to 30%. The activation energy of the Mg-acceptor E_{MG} and the Ni-Schottky barrier height of p-type AlGaIn $e\Phi_{\text{b}}$ was approximated by $E_{\text{MG}}(x) = (0.7 \text{ eV})x + 0.17 \text{ eV}$ [10,11] and $e\Phi_{\text{b}}(x) = (1.3 \text{ eV})x + 0.55 \text{ eV}$ [12], respectively, where x denotes the Al concentration in the barrier.

The calculated sheet density of holes is depicted in Fig. 1 as a function of the Al concentration, together with the magnitude of the transverse polarization charge. It can be clearly seen that the 2D hole density almost reaches the polarization charge density which implies that the latter never gets completely screened. The lower curves in Fig. 1 correspond to a fully strain relaxed AlGaIn layer, i.e., only the spontaneous polarization contributes to the interface charge. This corresponds to a situation where the barrier width exceeds its critical thickness. However, some experiments [3] indicate that there is a smooth transition from strained to relaxed barrier growth in a certain range of Al concentrations. This implies that the two curves in Fig. 1 should be

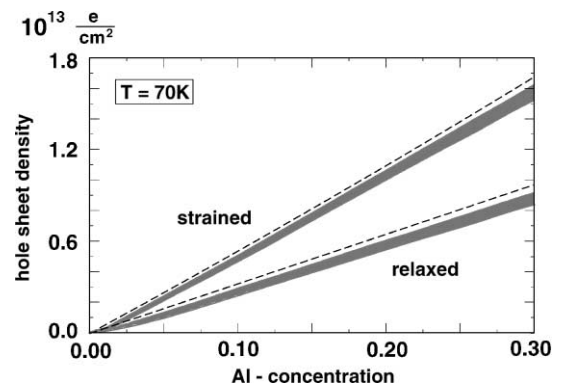


Fig. 1. Calculated hole sheet density for a gated strained (upper curves) and a gated relaxed GaN/AlGaIn heterostructure (lower curves) as a function of the Al concentration. The shaded contours mark the calculated densities for AlGaIn barrier widths in the range from 15 nm (lower edge of contours) to 35 nm (upper edge of contours). The dashed lines depict the magnitude of the polarization charge densities induced at the GaN/AlGaIn interfaces.

considered as limiting cases. Nevertheless, our calculations clearly demonstrate that the 2DHGs with hole densities of order of 10^{13} cm^{-2} can be achieved even in the fully relaxed structures. We would like to point out that the hole sheet density is quite insensitive to changes in other parameters such as temperature T , Schottky barrier height $e\Phi_b$, or valence band offset ΔE_V at the GaN/AlGaIn interface. We have verified this by systematically varying T (from 70 to 300 K), $e\Phi_b$ (by 50%), ΔE_V (from 0.25 to 0.6 eV), as well as the spacer width (from 0 to 5 nm). Each of these changes influences the hole sheet density by less than 5%.

As the second example for a possible source of high density 2DHGs, we have studied periodic GaN/AlGaIn superlattices at $T=70 \text{ K}$ with an aluminum concentration of 30% and various well (GaN) and barrier (AlGaIn) widths. In our calculations, we have assumed the barriers to be homogeneously p-doped with a Mg-concentration of $5 \times 10^{19} \text{ cm}^{-3}$, whereas the Mg-concentration in the well has been taken to be $1.6 \times 10^{17} \text{ cm}^{-3}$. The resulting hole sheet densities are shown in Fig. 2. It can be seen that the density is quite low for short well and barrier widths but increases and further saturates for thicker layers. These results can be understood from the spatial dependence of the acceptor level energies relative to the Fermi energy, which is depicted in Figs. 3 and 4 for thin and thick superlattice layers, respectively. In

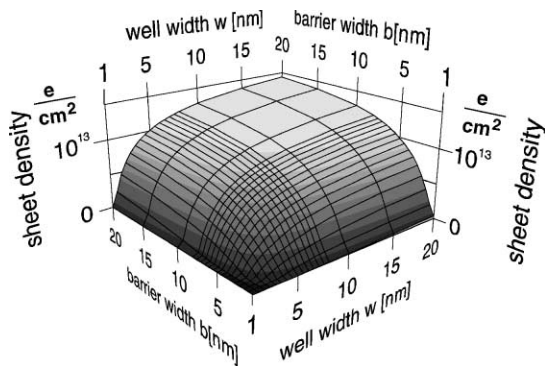


Fig. 2. Calculated hole sheet density of the GaN/AlGaIn superlattice with 30% Al concentration in the barriers as a function of the barrier (b) and well (w) widths in nm.

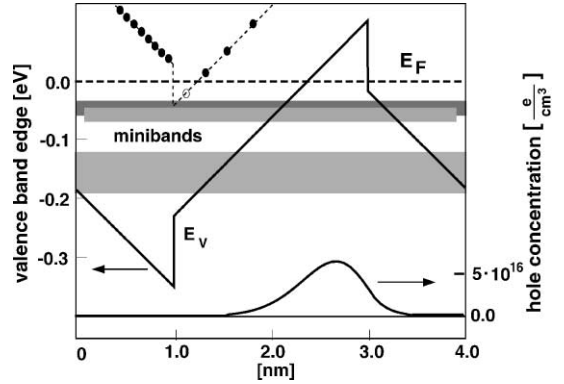


Fig. 3. Spatial dependence of the valence band edge E_V in the GaN/AlGaIn superlattice (30% Al content). The GaN well and AlGaIn barrier widths are equal to 2 nm. The dashed line indicates the position of the Fermi level. The energies of the neutral and ionized Mg-acceptor levels are indicated by full and open circles, respectively, and are connected by a dotted line to guide the eye. The shaded stripes show the position of the three topmost minibands. The corresponding density of the 2DHG is depicted in the lower part of the figure.

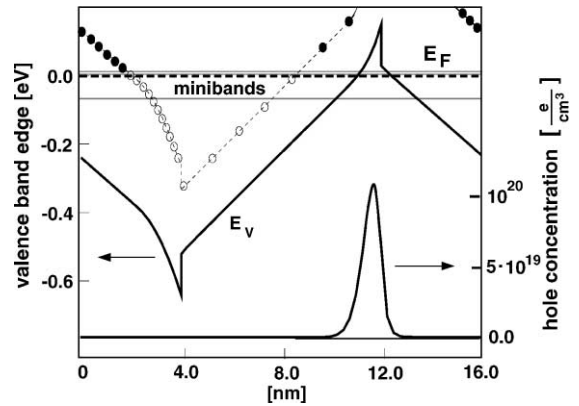


Fig. 4. Same as Fig. 3, but for a superlattice with GaN well and AlGaIn barrier widths equal to 8 nm.

superlattices, the polarization induced interface charges yield an intrinsic electric field of opposite sign in the GaN wells and the AlGaIn barriers. This variation causes a corresponding spatial sawtooth type dependence of the valence band edge. In short period superlattices, most of the Mg-acceptor levels do not fall below the Fermi energy (see Fig. 3). Accordingly, the hole density supplied by the acceptors is nearly zero in this case. By

contrast, in superlattices with thicker layers many acceptor levels are ionized (see Fig. 4). These ionized acceptors and the generated holes together screen the polarization charges and thereby diminish the intrinsic electric field. Consequently, the hole densities tend to saturate with increasing layer width. Our calculations predict a saturated hole sheet density of roughly $1.5 \times 10^{13} \text{ cm}^{-2}$ for GaN/AlGaN superlattices with 30% Al-concentration. We note that this density is similar to the hole density predicted for the heterostructure discussed above.

Our calculations provide additional information about the character of the confined hole spectra. In particular, Fig. 3 shows the minibands in the 4 nm period superlattice. The first miniband lies 35.8 meV below the Fermi level. Due to the short period, the overlap between hole wavefunctions from adjacent wells is considerable. Hence, we find fairly large widths of 23.56, 23.84, and 71.4 meV for the three topmost minibands, respectively. The two highest minibands considerably overlap and have strongly mixed heavy- and light-hole character while the lower miniband has dominantly split-off hole character. In the 16 nm period superlattice, on the other hand, the two uppermost minibands lie above the Fermi level (see Fig. 4), and all three bands have nearly a vanishing width of only 1.5 meV.

We have investigated additional possibilities to reach even higher 2DHG concentrations in GaN/AlGaN superlattices by optimally tailoring the doping profiles. Following a suggestion of Ref. [1], we have studied superlattices with a modulation doping profile where half of the well and half of the barrier surrounding the positively charged interface are homogeneously doped with $[\text{Mg}] = 5 \times 10^{19} \text{ cm}^{-3}$. Our calculations show that this profile increases the hole density particularly for short-period superlattices. To be specific, we find the hole density to increase from 3.9×10^9 to 5.2×10^{11} , from 7.7×10^{12} to 1.0×10^{13} , and from 1.4×10^{13} to 1.5×10^{13} for superlattices with periods of 4, 12, and 40 nm (equal well and barrier width), respectively. This dramatic change of the hole density for short period superlattice can be

explained with the help of Fig. 3. Since the region where the acceptors get ionized is very small for narrow superlattices, the 2DHG density linearly varies with doping concentration. By contrast, the hole density saturates due to screening effects for thick superlattice periods (Figs. 4 and 2).

In summary, our self-consistent calculations of GaN/AlGaN gated heterostructures and superlattices clearly demonstrate that one can achieve 2DHG densities of the order of $1.5 \times 10^{13} \text{ cm}^{-2}$ in both Mg-doped structures. This high hole sheet density is a consequence of the strong pyroelectric and piezoelectric character of wurtzite nitrides.

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