Piezoelectric Polarization in GaInN/GaN Heterostructures and Some Consequences for Device Design

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The polarization properties of doped Ga₀.₈₅In₀.₁₅N/GaN multiple quantum well structures are investigated under the application of external bias voltages. From Franz-Keldysh oscillations at and above the barrier band edge, the electric field in the barriers is determined. From the bias dependence, we derive the polarity and an offset of 0.51 MV/cm of the internal field. This is attributed to the piezoelectric polarization in the well region of magnitude $\vec{P} = +\varepsilon_z (0.009 - 0.014) \text{ C/m}^2$. We find that Si doping at typical concentrations of $3 \times 10^{18} \text{ cm}^{-3}$ cannot screen the polarization effects on the length scale typical for quantum wells and superlattices but induces large potential barriers.

KEYWORDS: GaN, GaInN, piezoelectric effect, electric field, Franz-Keldysh effect, electoreflection

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1. Introduction

Not only do significant ionic contributions in the covalent bonding forces of group-III nitrides lead to chemically stable and mechanically strong materials but, also, due to the uniaxial nature of the wurtzite lattice structure, the inversion asymmetry in compound semiconductors leads to very large polarization effects along the unique \( c \)-axis (0001) which typically coincides with the direction of the epitaxial layer and heterostructure growth \( \vec{z} = z \vec{e}_z \).\(^{1-5}\) The presence of large piezoelectric fields in strained GaInN/GaN heterostructures was first concluded from a quantum confined Stark effect in the photoluminescence (PL) of diode devices under variable bias\(^5\) and values for the fixed polarization field in the well could be derived.\(^6\) A more direct determination of internal field strength became possible by the observation of Franz-Keldysh oscillations (FKOs) in photomodulated reflection in strained GaInN layers.\(^7\) To quantify, and assess the polarity and effects of carrier screening on the polarization fields, we present electroreflectivity (ER) data in GaInN/GaN heterostructures and draw conclusions for device design.

2. Experimental

A GaInN/GaN multiple quantum well (MQW) structure was grown by metalorganic vapor phase epitaxy on (0001) sapphire. Atop a 2 \( \mu \text{m} \) GaN layer, a set of five \( L_w = 30 \) Å \( \text{Ga}_{0.85}\text{In}_{0.15}\text{N} \) wells were embedded in six \( L_b = 60 \) Å GaN barriers. The barriers of the structure were Si doped to \( N_D = 3 \times 10^{18} \text{ cm}^{-3} \). Electroreflectance was performed using an aqueous electrolyte and a C electrode. All measurements were performed at room temperature.

3. Results

Electroreflectance (ER) under variable bias voltage in the doped sample is presented in Fig. ??. An electric field is applied perpendicular to the doped MQW layer by two lateral top contacts. One of the contacts is formed by the transparent electrolyte. ER is measured around this contact. Negative bias voltages correspond to a lowering of the electron potential at the layer surface while positive voltages correspond to a depletion of the surface and extension of the field across the MQW thickness (see sketches in Fig.
Above an energy of 3.355 eV, strong FKO s appear in most of the spectra extending up to 3.940 eV (note the capped signal extrema in $E_i$ in this presentation). At lower energies, interference fringes appear as is apparent from the comparison with the DC reflection signal. Interpretation of the oscillation period along the approximation of the electro-optical functions results in a rather accurate reading of the electric field as shown by the good linear variation of $\frac{4}{3\pi} (E_i - E_0)^{3/2}$ vs the index $i$ of the extrema (inset of Fig. ??). In this interpretation, the joint density of state mass assumed at the GaN cyclotron resonance mass value $m^*/m_0 = 0.23$ is the only parameter.

We identify field values varying at a rate of $\frac{\partial F}{\partial U_{bias}} = 0.045 \text{ MV/cm/V}$ and a significant field value of $F_0 = 0.51 \text{ MV/cm}$ at zero bias voltage with reference to the C electrode (Fig. ??). The sign of the field can be derived to $\vec{F}_0 = +F_0 \hat{e}_z$. This reveals that even in the highly Si doped sample, significantly large electric fields are active without an external bias.

4. Discussion and Implications

The appearance of FKO s in photoreflection has previously been reported at energies below the GaN band edge and was associated with the GaInN layers. In this case, however, similar to the findings in ref. ?? oscillations appear only at and above the GaN band gap and the field must be assigned to the GaN barriers. An origin in the underlying undoped epilayer must be excluded because the contact with the sample is made only in the topmost MQW region. Despite the high doping conditions of the sample, the applied bias voltage can vary the electric field within an optical absorption length of 100 nm equivalent to the entire MQW region by an amount of $\Delta F_b = 0.36 \text{ MV/cm}$. Neglecting any contact losses, the geometrical field maximum is 2 MV/cm.

The existence of the finite field $F_0$ reveals a finite polarization within the structure. This has previously been assigned to the piezoelectric properties of the strained GaInN wells due to the pseudomorphic growth on GaN. In turn, an electric field in the barriers $\vec{F}_b$ is the direct response to polarization $\vec{P}$ and fields $\vec{F}_w$ within the wells according to $\vec{F}_{avg} (L_w + L_b) = \vec{F}_w L_w + \vec{F}_b L_b$ and for thermodynamical equilibrium $\vec{F}_w = -\vec{F}_b L_b/L_w = -2 \vec{F}_b$. The observation of the level splitting in the wells, how-
ever, suggests that $|\vec{F}_w| \approx |\vec{F}_b|$. This leads to the value of the piezoelectrically induced polarization $\vec{P} = -q_0 \varepsilon_v (\vec{F}_w - \vec{F}_b) = +\varepsilon_z (0.009 - 0.014) \, \text{C/m}^2$ or area charge accumulations of $\sigma = (5.9 - 8.8) \times 10^{12} \, \text{cm}^{-2}$ for Ga$_{0.85}$In$_{0.15}$N on GaN with $\vec{F}_b = \vec{F}_0$. First principles calculations$^{12}$ indicate that in contrast to the AlGaN/GaN system where the equilibrium polarization is thought to dominate, polarization in GaInN/GaN is attributed predominantly to piezoelectricity.$^2$ We therefore relate the polarization to the induced biaxial strain of the wells to obtain a piezoelectric coefficient $\partial P/\partial \varepsilon_{zz} = (0.92 - 1.43) \, \text{C/m}^2$. These values are higher than previously interpreted results in strained GaInN/GaN thin films$^7$ and below results obtained from piezoresistive measurements$^3$ in GaN and from first principles calculations$^4$ $\partial P/\partial \varepsilon_{zz} = 2.66 \, \text{C/m}^2$.

The role of screening of the polarization can be considered in the following approach. Dipole charges such as the piezoelectric polarization across the GaInN well can only be screened by charge carriers of both polarities. Such a situation exists in the spatial separation of free carriers from their fixed dopant charges. For effective mass-type donors with a typical dopant concentration of $3 \times 10^{18} \, \text{cm}^{-3}$, a full depletion length of 45 nm is needed to compensate $\sigma$ and an associated potential step would amount to 3.5 eV. Screening by doping of such a concentration can therefore not be achieved in typical quantum wells of 2 to 4 nm width and in the present sample the Si doping should not affect the interpretation by more than 10%. Moreover, the doping cannot be responsible for inducing the fields observed.

Screening therefore acts on the long range across the entire MQW region and compensates the built-up polarization to $\bar{F}_{\text{avg}} = 0$ for vanishing bias. For p-type doping, typical acceptor concentrations reach values of $5 \times 10^{19} \, \text{cm}^{-3}$ leading to screening lengths of the order of 1 nm which should allow a screening in quantum wells. The large binding energy of acceptors, however, would always result in a minimum potential of $E \approx 0.24 \, \text{eV}$ across the depletion length. In combination with spacer layers for remote doping, this step can easily hinder the transfer of holes into shallow wells for small InN fraction.

Screening should also be possible by bipolar injection of appropriate densities of free carriers under forward bias, i.e. at the lasing threshold. Values of $1 \times 10^{19} \, \text{cm}^{-3}$ equivalent to $3 \times 10^{12} \, \text{cm}^{-2}$ are, however, insufficient for complete screening even under the assumption
of a dipole length of the full well width. This is in agreement with recent band structure calculations.\textsuperscript{13} Therefore the most likely situation is a balancing of the dipole moments between doping layers and polarized layers along the above scheme. This indicates that polarization effects are important on a length scale typical for interfaces, heterostructures, superlattices, and intrinsic regions but not for general bulk applications. Within quantum wells, the polarization field induces level shift\textsuperscript{6} and level splitting\textsuperscript{12} which in turn is observed as a multitude of emission lines at different wavelengths.\textsuperscript{11,14}

5. Conclusions

From the interpretation of FKO\textsubscript{s} we directly determined the acting electric fields in the barriers of device typical GaInN/GaN heterostructures while previous results had been limited to the well regions only. By considering the balancing of polarization in wells and barriers, we derived values for the piezoelectric polarization $\vec{P} = +\vec{e}_z (0.009-0.014) \text{ C/m}^2$ for Ga$_{0.85}$In$_{0.15}$N/GaN. The numerical uncertainty is induced by the details of the balance between electric fields in the wells and the barriers. By applying an external bias voltage, the proper sign of the polarization was determined to point along the (0001) direction which coincides with the typical growth direction for metalorganic vapor phase epitaxy. We find that the polarization is little affected by a doping of the barriers with Si at a concentration of $3 \times 10^{18}$ cm$^{-3}$ due to the very high two-dimensional charge density of the piezoelectric polarization that resembles ideal $\delta$-doping layers. We conclude that screening by doping can only be active on a large length scale of several 10 nm to balance the average electric field but it is not a sufficient process to compensate the average polarization effects locally on the length scale of a few nanometers ($\sim$ 10 nm) across a quantum well. On the short length scale, the piezoelectric polarization was found to control the electronic band structure by field controlled shifts of the peak luminescence and the splitting of levels in interband absorption. The properties derived here for GaInN/GaN can be generalized to AlGaN, AlInN and other group-III nitride heterostructures by including the effects of spontaneous polarization in a similar manner.
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References

Figure captions

Fig. 1. Electroreflection in a doped GaInN/GaN MQW structure as a function of applied bias voltage. Above the GaN band gap, strong Franz-Keldysh oscillations appear with extrema in $i = 1 \cdots 7$. This allows a reading of the electric field and its direction with respect to the crystal orientation.
Fig. 2. Interpretation of the oscillation period (inset) and derived electric fields values.

The respective band edge diagram for both bias polarities is sketched. Besides very large electric fields, we identify a finite acting field at zero bias with respect to the C electrode. This field is the response of the piezoelectric polarization in the wells. From the linear variation of the field, we conclude that effects of doping at $N_D = 3 \times 10^{18}$ cm$^{-3}$ does not affect the field distribution significantly.