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

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1. Introduction

Significant ionic contributions in the covalent bonding forces of group-III nitrides do not only lead to chemically stable and mechanically strong material but due to the uniaxial nature of the wurtzite lattice structure the inversion asymmetry in compound semiconductors here leads to very large polarization effects along the unique *c*-axis (0001) which typically coincides with the direction of epitaxial layer and heterostructure growth [1,2,3,4,5]. To assess their role in the electronic bandstructure and band profile in optoelectronic GaInN/GaN heterostructures and devices we performed a variety of photomodulated reflectivity experiments and draw conclusions for heterostructure and device design.

The presence of large electric fields in pseudomorphically strained GaInN/GaN heterostructures was observed experimentally by the variation of the photoluminescence emission energy as a function of an externally applied bias voltage by Takeuchi *et al.* [5]. This behavior could be explained in terms of the quantum confined Stark effect and by comparison with band structure calculations values for the fixed polarization field in the well could be derived [6]. An even more direct experimental determination of the strength of internal electric fields and the associated polarization became possible by the observation of Franz-Keldysh oscillations in the photomodulated reflectivity in strained GaInN layers [7,8,9]. A similar observation in pseudomorphically strained GaInN/GaN multiple quantum well structures furthermore lead to a similar direct determination of polarization fields in the quantum well regions [10]. Here we compare the obtained experimental field values for various samples and results from first principles calculations in the literature [4]. From this we draw important conclusions and criteria for the device design in group-III nitrides with respect to this polarization effects.

2. Results and Discussion

Experimental electric field values derived from interpretations of Franz-Keldysh oscillations are collected in Fig. 1a) versus the InN molar fraction x. Collecting data from pseudomorphically strained GaInN/GaN films, and quantum well series with different composition and two different growth processes we observe a very general trend towards higher field for increasing x (right hand scale). At the same time, however, a significant variation in the data is seen. Results from theory are included as a dashed line on two different scales [4]. In the theory work the polarization was calculated in a number of nitride binaries as well as their strain derivatives, i.e. piezoelectric coefficients. The data presented here is based on the assumption of pseudomorphic growth of GaInN on GaN using linear interpolations of binary values.

We readily observe significant discrepancies between experiment and most importantly we find the opposite trend with x. In contrast to the scatter in this presentation of the data, a very clear correlation with little variation appears when the splitting of electronic levels in quantum wells [10] is considered as a function of the derived electric field. This strongly suggests that the quantity of the electric field, induced by the polarization charges is the crucial factor in the description of the optoelectronic properties. The large discrepancy between theory and experiment as well as the large variation of the experimental values as a function of x raise the question of possible unaccounted screening effects in the experimental results. We consider this in the following approach. For blue light emitters a composition of x=0.15 is typically chosen where we derive a field of 0.8 MV/cm corresponding to fixed piezoelectric area charges of $\sigma_{15} = 4.5\times10^{12}$ cm^{-2}.

The role of screening of the piezoelectric dipole charges can be considered in the following approach. Dipole charges like 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 homogenous dopant concentration of 2×10^{18} cm^{-3} a full depletion length of 45 nm is needed to compensate σ_{15}. Screening by doping of such concentration can therefore not be achieved in typical quantum wells of 2

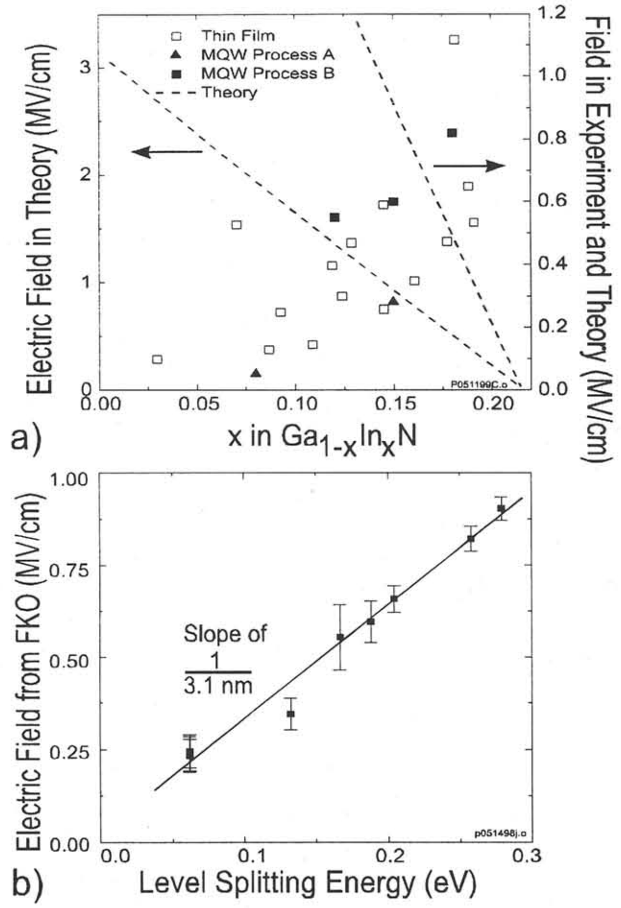

Fig. 1. a) Electric field in strained GaInN on GaN in experiment and theory. b) Correlation of level splitting and electric field.

to 4 nm width. For *p*-type doping the typical acceptor concentration reaches values of $5x10^{19}$ cm^{-3} leading to screening lengths of the order of 1.9 nm which theoretically would allow a screening in quantum wells. Screening should also be achievable by bipolar injection of appropriate densities of free carriers under forward bias, i.e. at the lasing threshold. Values of $1x10^{19}$ cm^{-3} equivalent to $3x10^{12}$ cm^{-2} are, however, insufficient for complete screening even under the assumption of a dipole length of the full well width. Such a dynamical screening furthermore renders the property of an inherently instable system which is very difficult to control and stabilize. Considering the two dimensional density of states in a QW with a typical depth of ΔE_c = 0.3 eV leads to $2.6x10^{13}$ cm^{-2} states for each spin-degenerate band. This is sufficiently large to accommodate an appropriate density of screening carriers.

All polarization that can not be screened locally will lead to band bending and charge rearrangement on a larger length scale. This includes the possibility to alter and control critical threshold voltages.

3. Conclusions

We have demonstrated that the quantity of the polarization in strained quantum wells and its associated fields are controlling the optoelectronic and bandstructure properties of GaInN/GaN heterostructures and a similar role must be expected in other group-III nitride heterostructures. We find that carrier injection and doping at typical dopant concentrations of $2x10^{18}$ cm^{-3} are insufficient to screen the fields in quantum wells in significant proportions. These arguments further show that screening under the considered conditions can also not account for the much larger field values that offset our results from the theory values. We must expect that the stabilization of internal electric field conditions should be very crucial for stable device performance.

Acknowledgments

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