Optical Properties of GaInN/GaN Heterostructures and Quantum Wells
C. Wetzel, T. Takeuchi, S. Nitta, S. Yamaguchi, H. Amano, and I. Akasaki
High-Tech Research Center & Dept. of Electrical and Electronic Engineering, Meijo University, Nagoya, Japan

Photoreflection and photoluminescence spectroscopies have been used to identify details of the electronic bandstructure in GaInN/GaN strained heterostructures and multiple quantum well structures. Franz-Keldysh oscillations in the ternary layers are identified in both systems revealing large piezoelectric fields of 240 kV/cm (x=0.079, thin film) and 0.65 MV/cm (x=0.187). From spatially resolved luminescence a very narrow distribution ΔE =28 meV of the bandgap energy is derived (x=0.187). From the variation of the field with strain a piezoelectric coefficient dPz/dε =0.3 C/m² is obtained corresponding to e14 = 0.1 C/m² and an equilibrium polarization of GaN of Peq =43 mCm² is extrapolated in qualitative agreement with recent calculations.

A. Introduction

Recent dramatic progress in alloys of group-III nitrides has led to high performance new devices such as short wave light emitting devices and high temperature and highest frequency field effect transistors [1]. Moreover, further progress is expected once the properties controlling the electronic bandstructure in thin films and quantum well structures is identified. The alloy of AlGaInN covers both a record in variation of the bandgap energy and in lattice constants. This advantage in the capability for bandgap engineering should therefore be coupled to challenges in stress design on heterostructures. Here we present the results of our recent studies in GaInN/GaN single and quantum well heterostructures.

B. Experimental

Samples in this study were prepared by metal organic vapor phase epitaxy on (0001) sapphire. Single 40 nm Ga1-xInxN/GaN heterostructures at various composition x (0<x<0.2) and multiple quantum well structures consisting of five 3 nm Ga1-xInxN wells embedded in 6 nm GaN barriers were studied by photoluminescence (PL) and photoreflection (PR) spectroscopy (T=300 K). Composition and stress conditions were analyzed by high resolution x-ray diffraction mapping of a and c lattice constants. A Xe-lamp white light source was used for PR measurements. Photomodulation was performed by a HeCd 325 nm laser. The same system was used for PL. Further details can be found in Ref. [2].

C. Single GaInN/GaN heterostructures

C.1. Stress and composition

The growth mode of this strongly lattice mismatched system GaInN/GaN was identified by x-ray mapping revealing pseudomorphic growth of the ternary layer at the a lattice constant of GaN. Despite the large thickness (40 nm) and the large lattice mismatch (∆a/a=1.1% for x=0.1) films were homogeneously strained under biaxial compression [3]. This result can not be explained by the current models of critical layer thicknesses in strained systems. This unexpected behavior strongly affects the interpretation of the In composition x from x-ray data. Assuming Vegard's law for the interpolation of the stress-free lattice
constant and linearly interpolated bulk moduli we find a relation between experimental \( c \)-lattice constant and \( x \) in the pseudomorphic system:

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x = 1.165 \left( \frac{c}{\text{Å}} - 5.184 \right) \left[ 1 - 0.16 \left( \frac{c}{\text{Å}} - 5.184 \right) \right] - 0.01; \quad a = 3.182 \text{ Å}.
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Herein, lattice constants \( c = 5.184 \) Å (5.705 Å), \( a = 3.188 \) Å (3.540 Å) and elastic constants (in \( 10^{11} \text{dyn/cm}^2 \)) \( c_{13} = 11.4 \) (9.4), \( c_{33} = 38.1 \) (20.0) in GaN (InN), respectively are used [4]. The constant offset originates in the stressed condition of the GaN reference layer. Consequently compositions derived without such a consideration overestimate the actual composition by roughly a factor of two. This may have contributed to discrepancies in the interpretation of results in the literature [5].

C.2. Luminescence bandgap in GaInN

Photoluminescence together with PR of a GaInN/GaN single heterostructure (\( x=0.18 \)) is presented in Fig. 1. Luminescence was excited with a spatial resolution of 1 \( \mu \text{m}^2 \) and mapped over an area of 50x50 \( \mu \text{m}^2 \). The spatial distribution of the peak center energy if given in Fig. 1.a). We find a center energy of 2.612 eV and a distribution with a halfwidth of only 25 meV. Weighing each peak energy position with the luminescence intensity we obtain the spectrum in Fig. 1.b) identifying the dominant emission energy at 2.620 eV at a distribution of 29 meV. The very good coincidence of both distributions indicates a very homogeneous distribution of the effective luminescence bandgap on the length scale relevant for optical emission. At the same time the PR spectrum (Fig. 1.c) shows a very broad oscillation in energy without any narrow (10-20 meV) features typically indicating the presence of excitons. In this data we furthermore find no evidence for a significant variation of the In composition at \( x=0.18 \). It has been proposed that apparent discrepancies in the expected transition energies are caused by the formation of In-rich islands or dots [6].

C.3. Piezoelectric field in GaInN

We assign the wide oscillation in the PR signal to Franz-Keldysh oscillations (FKO's) caused by an electric field across the ternary layer [7, 8]. Another PR spectrum for \( x=0.079 \) is given in Fig. 2.a). A clear minimum \( D_0 \) is seen in the vicinity of the GaInN bandgap. We recently used this to study the composition dependence of the bandgap energy [9]. Characteristic subsidiary oscillations (\( D_1 \ldots D_3 \)) can be identified on the high energy side (see also Fig. 1.c), \( x=0.18 \). An interpretation of the period according to

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**Figure 1.** Distribution functions of the maximum in spatially resolved photoluminescence. (a) Distribution of peak maximum. (b) Distribution of peak maximum weighed by its intensity. (c) Photoreflectance for comparison showing only Franz-Keldysh oscillations.
Aspnes [10] leads to a field value of 260 kV/cm (x=0.079) and a very high field of 0.65 MV/cm for x=0.187. We propose that this field is caused by piezoelectricity and strain in the non-centro-symmetric wurtzite structure. The polarization shows a trend to increase with composition or strain at an averaged rate of $dP_z/d\varepsilon_{zz}=0.3 \text{ C/m}^2$ corresponding to $e_{14} = 0.1 \text{ C/m}^2$ interpreting a set of 13 samples [11]. Considerable spread of the data indicates the presence of an effective field relaxation mechanism. Besides screening by mobile carriers domains of inverted crystal polarity may play a role. An extrapolation of the data indicates that the piezoelectric polarization should not vanish for vanishing strain but exhibit an offset corresponding to $|P_{eq}|=43 \text{ mC/m}^2$ of opposite direction. Such a behavior in GaN has recently been predicted in first principles calculations [12]. Values of $dP_z/d\varepsilon_{zz}$ and $P_{eq}$ found here however are only about 10% of the values predicted. The PR signal of the GaN layer underneath the ternary film does only reveal a third-derivative-like structure of the excitonic nature of the bandgap. We find no indications of the presence of an electric field across the GaN layer. This may be the result of an effective overall screening of the net field across the sample by charges and reconstruction on the surfaces to maintain the thermodynamic equilibrium. In turn no features indicating the dominance of excitons are observed in the PR signal of the GaInN layer. Applying the mechanism of Frenkel-Poole ionization excitons should be dissociated already at fields of 100 kV/cm.

D. GaInN/GaN multiple quantum well structures

PR of a multiple quantum well structure is shown in Fig. 2.b) [2]. We again identify excitonic contributions in the vicinity of the GaN excitonic bandgap of the buffer layers. In addition, however, there is an oscillatory contribution (peaks C$_0$ ... C$_4$) in the energy range above and below the GaN bandgap starting sharply at $E = 3.33 \text{ eV}$ in this structure. There is a strong resemblance with FKO's in the non-quantized thin films. An equivalent interpretation of the period results in an electric field value of 240 kV/cm. All extrema values excluding the ones associated with excitons in GaN are very well described using the approximate description or the electrooptical functions as given by Aspnes [10]. The mere superposition of the GaN signal rather than incorporation of it indicates that this field again does not apply to either the GaN epilayer, the barrier layers or both. Instead in these higher states of the GaInN
well the effect of FKO's dominate over the two-dimensional system. As a consequence the electric field can not be considered a weak perturbation in these states. At lower energies two more transitions $A$ and $B$ are identified (see Fig. 1.b). Level $A$ very closely corresponds to the luminescence maximum (Fig. 1.c)) and is tentatively assigned to the lowest quantized state in the quantum well system, while level $B$ corresponds to the first excited state. A detailed identification of both levels is underway.

E. Summary

In summary we have performed a spectroscopic analysis of the electronic bandstructure in $\text{Ga}_{1-x}\text{In}_x\text{N}/\text{GaN}$ thin films and multiple quantum well structures. A spatially resolved photoluminescence mapping reveals a very homogenous distribution of the InN fraction on the length scale of 1 to 50 $\mu$m resulting in a luminescence peak distribution of 25 meV ($x=0.18$). Franz-Keldysh oscillations were observed in both structure types identifying electric fields in the range of 260 kV/cm ($x=0.078$) and similar values in the quantum well case. In the case of a thin film sample of $x=0.187$ a maximum field of 0.65 MV/cm is observed. An average strain derivative $dP_z/d\varepsilon_{zz} = 0.3 \text{ C/m}^2$ corresponding to $e_{14} = 0.1 \text{ C/m}^2$ is observed.

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References