PIEZOELECTRIC QUANTIZATION IN GaInN THIN FILMS AND MULTIPLE QUANTUM WELL STRUCTURES

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ABSTRACT

Details of the electronic bandstructure in pseudomorphic $\text{Ga}_{1-x}\text{In}_x\text{N}/\text{GaN}$ single heterostructures ($0 < x < 0.22$) are studied. In photocarrier modulated reflectance strong modulation of the density of states (Franz-Keldysh oscillations) is found due to a piezoelectric field of about 0.6 MV/cm in the strained layer. No excitons are expected to form in the presence of this field. Studying the composition dependence we determine a piezoelectric coefficient $\partial P / \partial \epsilon_{zz} = 0.46 \text{ C/m}^2$ and extrapolate a spontaneous polarization in GaN $|P_{eq}| = 3.9 \text{ mC/m}^2$. Photoreflexion indicates the presence of localized tail states 50 - 100 meV below the bandgap which are well explained by the Franz-Keldysh effect involving k non-conserving transitions in the large electric field. Luminescence is found to originate in these electric field induced states. The derived bandgap energies can be approximated by an interpolation yielding bowing parameters $b = 2.6 \text{ eV}$ (photoreflexion) and $b = 3.2 \text{ eV}$ (luminescence) for pseudomorphic films with $0.07 \leq x \leq 0.22$. These findings may affect interpretation of device performance.

INTRODUCTION

Increasing economical relevance of group-III nitride based devices demands an thorough understanding of the electronic band structure and light emitting processes in this wide bandgap semiconductor system. Without closely matching substrate available the nitrides depend on epitaxial growth processes capable of bridging large lattice mismatch to i.e. 6H-SiC or sapphire. Here the development of low temperature deposited AlN [1,2] or GaN [3] buffer layers to accomplish lattice mismatch up to 14% between GaN and basal plane sapphire has laid the foundation for sophisticated bandstructure control by stress and its related phenomena such as piezoelectricity. In AlGaIn/GaN field effect device structures piezoelectricity was found to significantly enhance the free electron density in 2d transport channels [4]. Comparing the (free) lattice mismatch of GaN-AlN and GaN-InN significant piezoelectric effects must be expected for biaxially strained GaInN/GaN heterostructures [5]. Here we present a study of the electronic bandstructure in GaInN/GaN single heterostructures by photoreflexance (PR) in comparison with photoluminescence (PL) results.

EXPERIMENTAL

Single $\text{Ga}_{1-x}\text{In}_x\text{N}/\text{GaN}$ heterostructures with an InN fraction in the range of $0 < x \leq 0.22$ were studied. MOVPE samples were grown on (0001) sapphire substrates using low temperature deposited AlN buffer layers [6-7]. Ternary layers at a thickness of 40 nm were grown pseudomorphically onto 2 μm GaN.

Figure 1 Photoreflection of pseudomorphically strained 40 nm GaInN/GaN single heterostructures for 11 different InN-fractions x . Spectra are presented with respect to their dominant minimum assigned to the PR bandgap. Franz-Keldysh oscillations are seen above the bandgap. Weaker extrema are indicated with ticks.

PR at room temperature was performed using a Xe-arc lamp as a white light source. Modulation was performed by photoexcitation using a 40 mW 325 nm HeCd Laser. PL was performed using a 325 nm HeCd laser. The InN fraction x was determined from x-ray diffraction taking into account deformation of the unit cell in the stressed layers [6].

Figure 2 Two PR spectra compared to electro-optical functions $F(-\eta)$ and $G(-\eta)$ as function of η ($\hbar\Theta$ electro optical energy). The period of the PR signal is well reproduced including the minimum near $\eta=0$ indicating a negligible contribution of excitonic effects in the PR signal.

extremum is obvious. Furthermore there is a trend to larger oscillation period for higher InN-fraction.

Aspnes has given analytical expressions for the modulation of the dielectric function in the vicinity of a critical point in the density of states (DOS) under an electric field [9]. In dependence of the local dispersion in the critical point the PR-signal forming imaginary part ϵ_2 of the complex dielectric function was given in form of the electro-optical functions $F(\eta)$ and $G(\eta)$ each of which is a summation of Airy functions of the reduced energy argument $\eta = (\hbar\omega - E_g)/\hbar\Theta$, where $\hbar\omega$ is the photon energy and $\hbar\Theta$ the electro-optical energy related to the stationary electric field $F = (\hbar\Theta)^{3/2} 2\mu/e\hbar$ with $\mu = 0.2 m_0$ being the joint effective DOS mass assumed to be constant at the GaN value.

Interpretation of the extrema according to the formula given by Aspnes and Studna [10] results in a very good description of the oscillation extrema for large electric field values. In Fig. 2 two PR spectra are scaled to the electro-optic functions $F(-\eta)$ describing a positive dispersion

RESULTS AND DISCUSSION

The surprisingly large thickness (40 nm) of the unrelaxed layers may be attributed to strong ionic character of the group-III nitrides on the one hand and to the alignment of all directional bonds either close to the c-plane or exactly in c-direction in the wurtzite structure on the other hand.

Photoreflection

Photoreflection of 11 samples with different composition in the vicinity of the GaInN bandgap is presented in Fig. 1. For the ease of interpretation spectra are aligned in the dominant minimum of the PR signal. Reflection is found to be modulated over a very wide energy range of about 500 meV. Features of excitonic origin are typically limited to some 10 meV and can therefore not be assumed to dominate this signal. Additional oscillations on the high energy side are seen and have previously been assigned to Franz-Keldysh oscillations in the presence of an electric field [8]. As indicated by ticks for the weaker extrema the modulation period decreases for higher energy within each single spectrum. A direct correspondence of the higher order oscillations with the width of the main

Figure 3 Electric field derived from Franz-Keldysh oscillation versus c-lattice constant in biaxially strained GaInN. A slope corresponding to $\partial P/\partial \epsilon_{zz} = 0.46 \text{ C/m}^2$ and an offset corresponding to $|P|_{eq} = 3.9 \text{ mC/m}^2$ are found. Scales for derived strain and InN-fraction x are added.

This scheme is identical to considering the variation of the bandgap in the electric field across the dimension of the particle of finite size, i.e. the electron-hole pair [8].

Piezoelectric Field

Analyzing all samples in the above scheme we derive the dependence of the net electric field F present in the ternary layer as a function of the c-lattice constant (Fig. 3). Scales for the derived ϵ_{zz} strain and the x are given. F increases with ϵ_{zz} corresponding to a piezoelectric constant $\partial P/\partial \epsilon_{zz} = 0.46 \text{ C/m}^2$ (slope indicated by dashed line). The typical maximum field observed is $\approx 0.6 \text{ MV/cm}$. In one case a field of 1.1 MV/cm is found. The large field value must be attributed to the net static piezoelectric field in the structure. The piezoelectric field extrapolates to zero field for finite strain ($\epsilon_{zz} = +0.0045$) or finite InN fraction ($x = 0.063$). Extrapolating further to the epitaxial GaN underneath the ternary layer an equilibrium polarization $|P_{eq}| = 3.9 \text{ mC/m}^2$ ($P_{eq} \partial P/\partial \epsilon_{zz} < 0$) is derived. We note that this minimum in polarization closely coincides with the composition of most efficient laser devices indicating that loss process may be induced by the field. The derived values are net fields as they may in part be screened by mobile carriers. The requirement of stationary boundary conditions at all times

in k_x , k_y , and k_z and $G(-\eta)$ appropriate for positive dispersion in k_x , k_y , and negative in k_z -direction. E_g in the calculated functions is identified with a dashed line. For the oscillating part above E_g very good agreement is found. In the range below E_g contributions from function $G(-\eta)$ in part give a better description of the data than function $F(-\eta)$ alone. There is good agreement also with the locations and relative intensity at the global minimum of the spectra close to the theoretical bandgap and this supports our interpretation that no excitonic contributions are seen in these spectra. Instead all features seen near and above E_g are described solely by Franz-Keldysh modulation of the DOS.

We propose that the contributions corresponding to a negative dispersion in k_z originate in the tilted bandstructure due to the large electric field leading to bandstructure extrema for finite k_z . This effective bandgap lowering is accessed by transitions involving particles of finite size or scattering partners such as phonons. It therefore corresponds to electric field induced localized states as well described by the Franz-Keldysh effect. For $F = 0.6 \text{ MV/cm}$ a redshift of the bandgap of 160 meV is expected [11].

Figure 4 Apparent bandgap in pseudomorphically strained $Ga_{1-x}In_xN/GaN$ as a function of InN fraction taking into account deformation of the unit cell. For $0.07 \leq x \leq 0.22$ effective bowing parameters can be given for the PL bandgap and the PR bandgap.

Luminescence typically emphasizes localized states over absorption-type measurements such as PR and an energetic separation between both results is expected. As pointed out in Ref. [8] luminescence maxima and PR maxima below E_g closely coincide in agreement with our discussion of the electric field induced localized states. Bandgaps can be interpolated with a bowing parameter b for the stressed system. For $0.07 \leq x \leq 0.22$ a good description is obtained for $b = 3.2$ eV, (PL), $b = 2.6$ eV (PR).

SUMMARY

An analysis of the electronic bandstructure of pseudomorphic GaInN/GaN heterostructures was performed by photoreflection spectroscopy. Large piezoelectric fields up to 0.6 MV/cm (typical) or 1.1 MV/cm (in one case) was found as a function of alloy-induced biaxial strain in the ternary layers. Due to Frenkel-Poole ionization no excitons are expected to form in the presence of this field. From a large number of samples with various composition an effective piezoelectric coefficient was derived and a value of the spontaneous polarization in GaN extrapolated. Compared to theoretical predictions significantly smaller values are found that in part may be attributed to screening by mobile carriers and defect formation. Identical electrical field conditions must be expected in GaInN/GaN quantum well structures with significant effects

including growth is expected to compensate any macroscopic field. We therefore expect a piezoelectric modification of the surface potential to affect growth and reconstruction properties. Additional bandoffsets in heterostructures, however, allow for a stabilization of a local electric field and its observation through Franz-Keldysh oscillations.

A first principles calculation of the polarization properties of group-III nitrides has recently been performed by Bernardini *et al.* [12]. Large piezoelectric constants and piezoelectric polarization have been predicted for GaN, AlN and InN. Comparing with our results these values for GaN are larger by a factor of 5 to 7: $\partial P / \partial \epsilon_{zz} = 2.37$ C/m² and $P_{eq} = -29$ mC/m². The discrepancies may in part be attributed to mobile carriers and piezoelectricity induced defect formation during growth.

From these PR data an effective bandgap for the stressed layers may be derived from the dominant minimum in PR. Data versus the InN-fraction are presented in Fig. 4 together with PL peak maxima energies.

on the bandstructure of devices. Large fixed piezoelectric charges induced at the interfaces act as δ -doping layers that cannot be screened entirely by carrier injection.

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