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CONTACTLESS ELECTROREFLECTANCE AND PIEZOREFLECTANCE OF A TWO-DIMENSIONAL ELECTRON GAS AT A GaN/AlGa_N HETEROINTERFACED.Y. Lin,^a Y.S. Huang,^{a,*} Y.F. Chen^b and K.K. Tiong^c^aDepartment of Electronic Engineering, National Taiwan University of Science and Technology, Taipei 106 Taiwan, People's Republic of China^bDepartment of Physics, National Taiwan University, Taipei 106, Taiwan, People's Republic of China^cDepartment of Electrical Engineering, National Taiwan Ocean University, Keelung 202, Taiwan, People's Republic of China

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We have measured the contactless electroreflectance and piezoreflectance spectra at 300 and 20 K from a GaN/AlGa_N heterojunction structure grown by metalorganic chemical vapor deposition on 6H-SiC substrate. The features related to a two-dimensional electron gas confined at the GaN/AlGa_N heterojunction are observed and the origin and nature of these features are discussed. © 1998 Elsevier Science Ltd. All rights reserved

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The properties of III–V nitrides have attracted great interest owing to their potential for blue and green light-emitting diodes [1], short wavelength lasers [2] and electronic devices for high power and high-temperature applications [3]. The high saturated drift velocity of electrons in GaN, combined with the large sheet densities and high mobilities attainable in GaN/AlGa_N enable improved performance for GaN-based devices in high power microwave applications [4]. Previous study in this area has confirmed the existence of a two-dimensional electron gas (2DEG) at the GaN/AlGa_N heterointerface [5, 6]. GaN/AlGa_N high electron mobility transistors (HEMTs) with high transconductances and promising d.c. and microwave operating characteristics have also been recently demonstrated [4, 7].

In this article we report the contactless electroreflectance (CER) and piezoreflectance (PzR) study at 300 and 20 K on a GaN/AlGa_N heterointerface. Sharp spectral structures associated with the intrinsic free excitons are observed by PzR measurement from the GaN region. The features corresponding to the Al_xGa_{1-x}N also yield the Al composition with $x = 0.16$. In both the PzR and CER spectra, we

observed derivative-like features related to a 2DEG confined at the GaN/AlGa_N heterointerface. The physical origin of these structures are analyzed through a self-consistence calculation. The sheet carrier density at the interface is evaluated and the results agreed well with the Shubnikov–de Haas (SdH) measurements [8].

The sample used in this study was grown by metalorganic chemical vapor deposition (MOCVD) on 6H-SiC substrate. Five periods of GaN/AlGa_N superlattice with total thickness of 1000 Å was introduced to accommodate the lattice mismatch with the substrate. This was followed by a wide GaN layer of 1.3 μm, capped with 500 Å AlGa_N barrier and 100 Å GaN top layer. Through out the crystal growth, no intentional doping was incorporated. The SdH measurements of the same sample was previously performed [8]. In the SdH measurement, a temperature independent mobility, indicative of the presence of a 2DEG, was observed in the sample below 77 K and a 2DEG mobility of about 4800 cm²/Vs, with sheet carrier density of 6×10^{12} cm⁻² at 4.2 K were obtained.

The CER technique utilizes a condenser-like system consisting of a thin indium tin oxide (ITO) on a quartz substrate which serves as an electrode. A second electrode consisting of a metal strip is separated from the first electrode by insulating spacers. The sample is

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placed between these two capacitor plates. Thus there is nothing in direct contact with the front surface of the sample. The dimensions of the spacers such that there is a very thin layer (~ 0.1 mm) of air (or vacuum) between the front surface of the sample and the conducting part of the first electrode. An a.c. modulating voltage (~ 500 V peak-to-peak) at a frequency of 220 Hz was employed. The variations of the field strength applied on the sample was estimated to be $\sim 3 \times 10^3$ V/cm. The CER approach has a number of advantages over photoreflectance for the study of wide-band-gap nitride samples. It does not require a UV laser as the pump beam and also avoids any photoluminescence background due to this pump beam [9]. A 150 W xenon arc lamp filtered by an Oriel model 257 monochromator provided the monochromatic light. The reflected light was detected by an EMR model 541E photomultiplier tube (PMT). The d.c. output of the PMT was maintained constant through out the experiment by an electronic servo which controls the high voltage applied to the PMT. The signal was recorded by an NF model 5610 B lock-in amplifier. The PzR measurements were achieved by gluing the sample on a 0.15 cm thick lead-zirconate-titanate piezoelectric transducer driven by a 200 V_{rms} sinusoidal wave at 200 Hz. The alternating expansion and contraction of the transducer subjects the sample to an alternating strain with a typical rms $\Delta l/l$ value of $\sim 10^{-5}$.

The CER and PzR spectra at 300 and 20 K are shown in Figs 1 and 2, respectively. In all of these spectra, we observe features which can be classified as GaN related, 2DEG related and AlGa_N related features. The GaN features are located at the low energy side while the AlGa_N features are at the high energy end. The 2DEG related features are marked with dotted enclosure and located in the intermediate energy range.

Fig. 1. The experimental CER spectra (solid curves) at 300 K (upper curve) and 20 K (lower curve). The open circles are least-squares fits to the first derivative of a Lorentzian profile, which yield the interband excitonic transition energies of AlGa_N. The dotted enclosure marks the 2DEG related features.

Fig. 2. The experimental PzR spectra (solid curves) at 300 K (upper curve) and 20 K (lower curve). The open circles are least-squares fits to the first derivative of a Lorentzian profile, which yield the interband excitonic transition energies of GaN. The 2DEG related features are also marked with dotted enclosure.

In the CER spectra, the broad structure at the low energy side is assigned to be GaN related. This assignment will be confirmed by the PzR spectra which are shown in Fig. 2. In Fig. 2, the PzR spectra were obtained for the sample at 300 and 20 K. For PzR spectrum at 20 K, the sharp spectral structures referred to as A, B and C excitons are respectively related to the $\Gamma_9^v - \Gamma_7^c$, $\Gamma_7^v - \Gamma_7^c$ (upper band)- Γ_7^c and Γ_7^v (lower band)- Γ_7^c interband transitions of GaN. The energy positions of these transitions are determined to be 3.477, 3.487 and 3.498 eV, respectively. We note that the values of the transition energies obtained here are lower than those reported in the literature, for example, 3.484, 3.49, 3.512 eV for GaN on sapphire substrates [10]. Such discrepancy can be attributed to the fact that the overall effects of residual strain generated in GaN on sapphire is compressive [11], while the stress induced in GaN on SiC is tensile [12].

In both the CER and PzR spectra, we also observed features at high energy end which are attributed to the band to band free exciton transitions of the AlGa_N. The structures are being fitted to the first derivative of a Lorentzian profile [13] and the transition energies are determined to be 3.76 and 3.83 eV at 300 and 20 K, respectively. The Al composition deduced from the expression [13] $E_{\text{Al}_x\text{Ga}_{1-x}\text{N}} = E_{\text{GaN}} + 1.75x + 0.98x^2$ with $E_{\text{GaN}} = 3.44$ eV yields $x = 0.16$. The oscillation-like features observed in PzR spectra (Fig. 2) for the photon energy range below the energy gap of GaN result from multilayer interference.

In Figs 1 and 2, we have also observed two broad features located in between the GaN and AlGa_N related structures. These features are high-lighted with dotted enclosure and are attributed to the 2DEG confined at the GaN/AlGa_N heterojunction. The onset of one of the

Fig. 3. The schematic band diagram at the GaN/AlGaIn heterointerface. The energy levels labeled as E_1 and E_2 are obtained from a self-consistent calculation. Also shown are the electron probability distribution of E_2 and the transitions taking place near the maximum probability positions in the 2DEG region.

features is slightly above the energy gap of GaN while the other peak is located slightly below the energy gap of AlGaIn. In order to explain the origin of these features, we utilized a model for the heterojunction structures which is similar to that of [14]. From the model, a schematic band diagram of the heterointerface is constructed and shown in Fig. 3. A self-consistent calculation of the energy levels at the heterointerface is performed. In the calculation we have used an electron effective mass of 0.25 of the free electron mass m_0 , a GaN energy gap of 3.44 eV, an AlGaIn energy gap of 3.76 eV and a conduction band offset coefficient, $Q_c = 0.80$ [15]. The electron effective mass is deduced from the temperature dependent SdH measurements [8] and the energy gap of AlGaIn is deduced from the measured spectra at 300 K. The proposed model does not account for many body effects, such as band-gap renormalization. The Fermi level in the GaN is assumed to be determined by shallow donors with $E_D = 42$ meV [16]. Although the sample is unintentional doped, in the majority of cases the AlGaIn growths are mainly degenerate n type ($N_d = 10^{18} \sim 10^{20} \text{ cm}^{-3}$) [17]. The sheet carrier density in the 2DEG is dependent on the carrier concentration in the AlGaIn layer. The experimentally measured electron concentration of $6 \times 10^{12} \text{ cm}^{-2}$ was obtained with a carrier concentration of $2 \times 10^{19} \text{ cm}^{-3}$. Under this condition two quantum confined states of the conduction band are obtained. The obtained states are E_1 (ground state) and E_2 (the first excited state) with energies 153 and 219 meV above the bottom of the potential notch, while the Fermi level is 206 meV above the potential notch. Under this situation, the Fermi level is higher than E_1 but slightly lower than

E_2 , the ground energy subband will be almost fully occupied while the first excited energy subband will be partially occupied by electrons transferred from the AlGaIn layer. This charge transfer gives rise to a negative space charge region on the GaN side of the heterojunction resulting in a built-in electric field in the direction normal to the heterojunction plane. The concentration of 2DEG could be estimated by [18]

$$N_s = \left(\frac{m_e^* k T}{\pi \hbar^2} \right) \sum_n \ln \left[1 + \exp \left(\frac{E_F - E_n^c}{k T} \right) \right] \quad (1)$$

where E_n^c is the n th electronic level in the 2DEG region, E_F is the Fermi level, m_e^* is the electron effective mass, k is the Boltzmann constant. In this case the 2DEG concentration is about $7.7 \times 10^{12} \text{ cm}^{-2}$ at $T = 300$ K. In equation (1), if we assume $E_F - E_n^c$ is independent of temperature, we obtain $N_s = 6.2 \times 10^{12} \text{ cm}^{-2}$ at $T = 20$ K. This value matches very well with the SdH results [8].

The origin of the two broad 2DEG related features can be understood as follows: the carrier concentration N_s of the 2DEG system was modulated as a result of a perturbation of the Fermi level with respect to the quantum confined states in the conduction band. However, since the Fermi level is higher than E_1 and close to E_2 , the ground subband is always full whether the external modulation is present or not. Variations of the carrier concentration and the imaginary part of the dielectric function (ϵ_2) due to the external modulation mainly resulted from the energy variation of the Fermi level with respect to E_2 . The ϵ_2 originates from the electrons in the extended 3D valence band to the subbands in the 2D region of conduction band can be expressed as [19]

$$\epsilon_2 \propto \left[\sum_{k_{\parallel}} |\langle v|s \rangle|^2 |\hat{e} \cdot \mathbf{P}|^2 \delta[E_2(k_{\parallel}) - E_v(k_{\parallel}) - \hbar\omega] \right] [1 - f_e(E_s)] \quad (2)$$

where $k_{\parallel}$ is the component of the wave vector paralleled to the surface and the summation is taken over the unoccupied conduction-subband states, $\mathbf{P}$ is the matrix element of the momentum operator with the Bloch states of the crystal and $\hat{e}$ is the polarization vector of the incident light, $f_e(E_s)$ is the Fermi-Dirac distribution with $E_s = E_2 + (\hbar^2 k_{\parallel}^2 / 2m_e^*)$, $\langle v|s \rangle$ is the overlap integral of the hole and electron functions on the valence and conduction subband, respectively. The square of the normalized envelope function which is proportional to the electron probability distribution of E_2 are also shown in Fig. 3. The probability distribution of the first excited subband as a function of position consists of two asymmetric lobes. The narrower lobe has its maximum near the heterointerface of GaN/AlGaIn whereas the

broader lobe extends out from the minimum of the narrower lobe to approximately the point where the E_2 subband energy level crosses the conduction band. Because the 3D valence band has a band bending on the negative space charge region while the two-dimensional subband energy level is a constant, the transitions originate from different positions along the extended 3D valence band required photons with different energies. Combining the effects of transitions from the valence band with a monolithically decreasing band bending to the conduction subband of 2DEG with a constant quantized level and the electron probability as a function of position, we can deduce that the change in ϵ_2 will give rise to two structures at different photon energy. The modulated intensity of the reflected light in a CER or PzR experiment is proportional to the superposition of the modulation of the real and imaginary parts of the dielectric function which are related by Kramers–Kronig relations. From the analysis, we can conclude that the broad peak on the low energy side of the 2DEG related features correspond to the transitions taking place from the valence band near the flat band region of GaN to the first excited energy subband. The location of the broad peak is estimated to be 3.5 ± 0.01 eV at 20 K. By the same reasoning, the narrower feature located at 3.725 ± 0.005 eV for spectra at 20 K is related to the transitions taking place from the valence-band states near the heterointerface to the first excited energy subband. The theoretical value of $E_{\text{GaN}} + E_2$ is equal to 3.72 eV which agrees well with the experimental data of 3.725 ± 0.005 eV.

In conclusion, we have measured the CER and PzR spectra from a GaN/AlGaIn heterojunction structure at 300 and 20 K. These results can provide the direct information about the AlGaIn band gap and hence Al composition of the AlGaIn layer is determined to be 0.16. Two broad features observed at the photon energy range between the GaN and AlGaIn band gap are strongly correlated to the presence of a 2DEG. Their origin and nature are discussed. A consistent result has been demonstrated by a self consistent calculation and the sheet carrier density at the interface is determined to be $6.2 \times 10^{12} \text{ cm}^{-2}$ at 20 K.

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