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Two-dimensional electron gas in cubic $Al_xGa_{1-x}N/GaN$ heterostructures

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We report on the optical and electrical properties of cubic $Al_xGa_{1-x}N/GaN$ heterostructures. The optical properties were investigated by photoluminescence measurements. A luminescence band at 3.250 eV was observed with our cubic $Al_xGa_{1-x}N/GaN$ heterostructures. The emission lies between the excitonic emission of c-GaN at 3.276 eV and the donor-acceptor transition at about 3.135 eV. With increasing excitation power we find a characteristic blue shift of 4.5 meV/decade. To confirm the existence of a two-dimensional electron gas the transition energy versus externally applied voltage has been investigated. A 1.3 meV/V shift was measured and quantitatively verified by a self consistent solution of the Schrödinger and Poisson equation. The electrical properties were determined by capacity-voltage (CV)-measurements. The measured carrier profile is in excellent agreement with theoretical simulations and showed a sheet carrier concentration up to $n = 1.6 \times 10^{12}$ cm^{-2} at the $Al_xGa_{1-x}N/GaN$ interface.

1 Introduction

The absence of spontaneous and piezoelectric polarization fields in cubic phase group-III nitrides avoids the severe red shift of quantum well emission energies and the strong reduction of the internal quantum efficiency observed with group-III nitrides with hexagonal crystal symmetry grown on c-plane substrates. Further, the density of the two-dimensional electron gas (2-DEG) in cubic $Al_xGa_{1-x}N/GaN$ heterostructures is independent on the thickness and Al mole fraction of the $Al_xGa_{1-x}N$ barrier layer and can be controlled by doping with silicon. Therefore, cubic GaN and its alloys have a lot of potential for the future use in electronic devices. However, the study of optical and electrical properties on cubic based $Al_xGa_{1-x}N/GaN$ heterostructures has been limited due to the difficulty to grow phase pure cubic GaN with a high quality interface and the lack of appropriate semi-insulating substrates. In wurtzite $Al_xGa_{1-x}N/GaN$ heterojunctions the existence of a 2-DEG is well known [1–3], but the presence of the internal electric fields allows only a restricted control of the 2-DEG channel. The existence of a 2-DEG in the cubic nitrides is only scarcely investigated [4], and for cubic nitrides any optical characterization of the $Al_xGa_{1-x}N/GaN$ interface is missing.

2 Experimental

Cubic $Al_xGa_{1-x}N/GaN$ heterostructures were grown on highly conductive 3C-SiC (001) substrates by plasma assisted molecular beam epitaxy [5]. The thickness of the c-GaN and c-$Al_xGa_{1-x}N$ epilayers were 1000 nm and 40 nm, respectively. The Al mole fraction was varied between x = 0.2 and 0.55. The barrier

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layer was capped by a GaN layer with different thicknesses between 0 nm and 20 nm. The unintentionally doped GaN and AlGaN epilayers have a free electron concentration of $2x10^{17}$ cm^{-3} and $2x10^{18}$ cm^{-3}, respectively. One of the essential parameters for the formation of a two-dimensional electron gas (2-DEG) is a low interface roughness. Using a special designed process for the growth of $Al_xGa_{1-x}N$ we were able to observe RHEED oscillations with the start of the growth [6] indicating a high quality of the interface. The optical properties were determined by photoluminescence (PL) measurements taken at T = 2 K varying the excitation power of the HeCd-laser between 0.2 Wcm^{-2} and 20 Wcm^{-2}. For bias dependent PL measurements a semitransparent contact was prepared on top of the GaN cap layer after cleaning the surface by organic solvents and a buffer oxide etch (BOE). A 5 nm thick, square shaped (1x1 mm^2), semitransparent Ni-Schottky contact was fabricated by thermal deposition and contact lithography. At one corner this semitransparent contact was mechanically reinforced by additional Ni/Au metal layers (45 nm/50 nm) with a diameter of 300 µm for easy bonding. Pure In contacts were used for the ohmic contacts to the 3C–SiC substrate. The applied bias voltage was varied between –1.5 V and 1.5 V. For CV measurements additional Ni/In (50 nm/150 nm) Schottky contacts with 300 µm diameter were used. The CV measurements were performed with a Boonton 72B bridge operating at 1 MHz between 0 V and -5 V in the temperature range from 5 - 350 K.

3 Results and discussion

Low temperature PL spectra of a cubic GaN epilayer and an $Al_{0.2}Ga_{0.8}N$/GaN heterostructure with an $Al_{0.2}Ga_{0.8}N$ thickness of 100 nm are shown in Fig. 1. In the spectrum of the heterostructure (Fig. 1b) a clear peak at about 3.250 eV is observed in addition to the well known excitonic transition at E_X = 3.276 eV and the donor acceptor transition at E_{DAP} = 3.134 eV of cubic GaN, respectively [7]. Previous study of the AlGaAs/GaAs system have shown an optical emission process, referred to as the H-band, which has been related to the recombination of confined and free carriers near the interfacial band bending region [8]. This H-band is characterized by a blue shift proportional to the logarithm of excitation power density due to the changes in energy band bending and shows a typical bias dependence.

For the investigation of the 2-DEG we have measured the photoluminescence at T = 2 K at different excitation powers. In the left side of Fig. 2 different spectra are plotted in the energy range from 3.2 eV to 3.3 eV. The spectra are normalized to one and they are linearly shifted for a better overview. With increasing excitation power the additional line at an energy of 3.250 eV shows a clear blue shift. In the right side of Fig. 2 the peak energy position is plotted versus the excitation power. A logarithmic increase of the peak position with increasing excitation power from 3.249 eV at a power of 0.2 Wcm^{-2} to 3.258 eV at 20 Wcm^{-2} is measured. A fit reveals a shift of 4.5 meV/ decade. This effect can be attributed to the recombination of electrons trapped in the potential notch next to the interface caused by the band-bending there with free holes in the valence band at some distance away from the heterointerface. The power dependence of the emission energy is explained as a result of photoexcited carrier screening of the built-in heterointerface field. This screening drives the band structure “flat band” and causes a blue-shift of the emission energy, which is proportional to the logarithm of the excitation power [9].

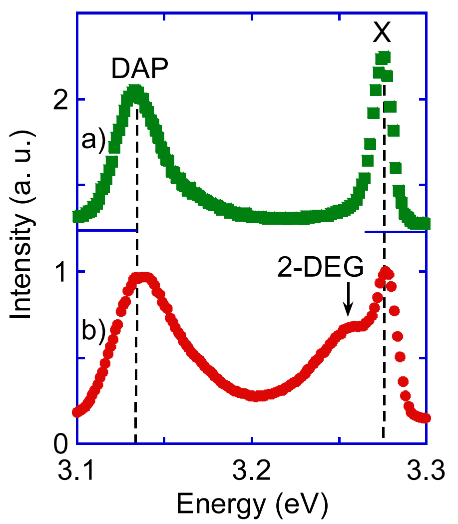

Fig. 1 PL spectra measured at T = 2 K for a bulk GaN layer (a) and an $Al_{0.2}Ga_{0.8}N$/GaN heterostructure (b).

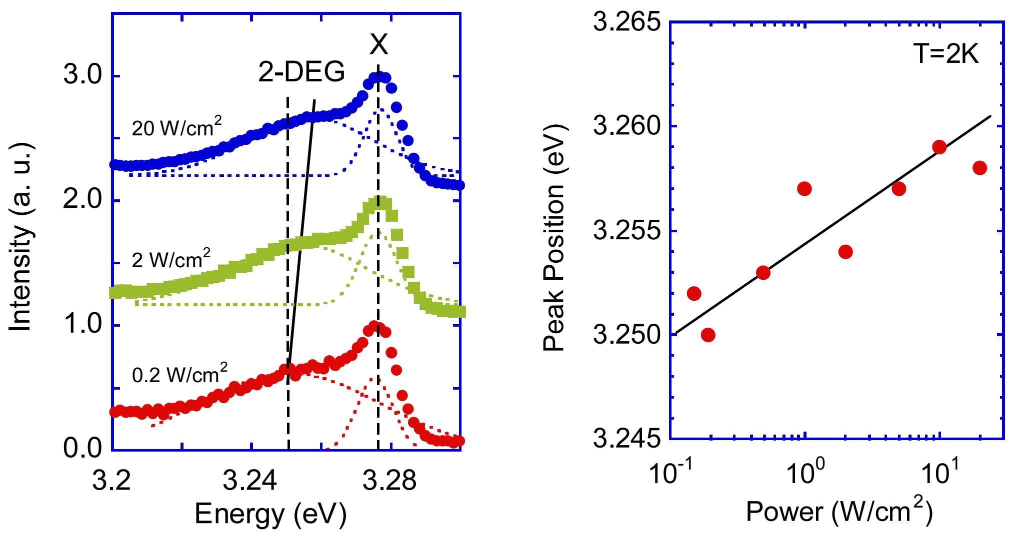

Fig. 2 Left side: PL-spectra of an $Al_{0.2}Ga_{0.2}N$/GaN heterostructure at T = 2 K at different excitation powers between 0.2 Wcm^{-2} and 20 Wcm^{-2}. Right side: Peak position of the 2-DEG correlated transition as a function the excitation power.

A direct experimental proof of this assignment to an H-band like transition is obtained by applying a weak electric field parallel to the growth direction. Such experiments were performed by applying an electric field parallel to the growth direction via a semitransparent Ni-Schottky contact. A clear blue shift in the energy position of 4 meV is observed by changing the bias voltage from -1.5 V to 1.5 V, which is plotted in Fig. 3. The shift of the transition energy can be explained by the variation of the band structure due to different applied external voltages. The shape and the depth of the potential well will change, which results in a shift of the quantization energy level of the 2-DEG. This change in energy level leads to a blue shift of the energy for positive biases and a red shift for negative biases in accordance with our observations shown in Fig. 3. The full black line in Fig. 3 is a guide for the eye.

On the left-hand side of Fig. 4 the band diagram and the electron density distribution is plotted versus depth for a cubic $Al_xGa_{1-x}N$/GaN heterostructure. The calculation was performed with a program, which solves in a self-consistent way the one-dimensional Poisson and Schrödinger equations [9]. For the unbiased case the Fermi-energy is depicted by the dashed horizontal line and the course of the conduction band energy E_c is indicated by the solid red line. As clearly can be seen a quantized energy level is formed at the $Al_xGa_{1-x}N$/GaN interface about 50 meV below the Fermi-energy. Taking into account that the band gap of cubic GaN is 3.304 eV and that the position of the Fermi-level is nearly identical with E_c a transition energy of about 3.250 eV is expected for the H-like band in c-GaN at 2 K, in excellent agreement with our observation. The corresponding electron density distribution is also depicted in the left side of Fig. 4 (dotted curve) indicating the formation of a two-dimensional electron gas between 60 nm and 64 nm with a peak carrier concentration of about 1×10^{19} cm^{-3}, just beneath the heterojunction.

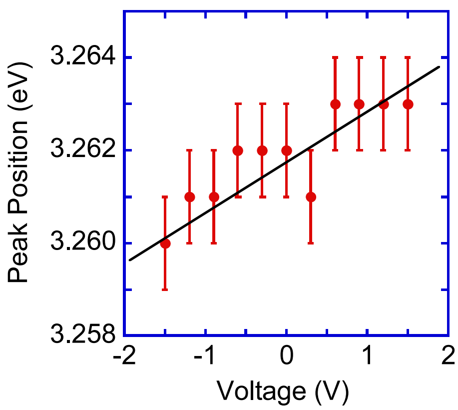

Fig. 3 Peak position of the 2-DEG transition at externally applied bias between -1.5 V and +1.5 V of an $Al_{0.2}Ga_{0.8}N$/GaN heterostructure at T = 2 K.

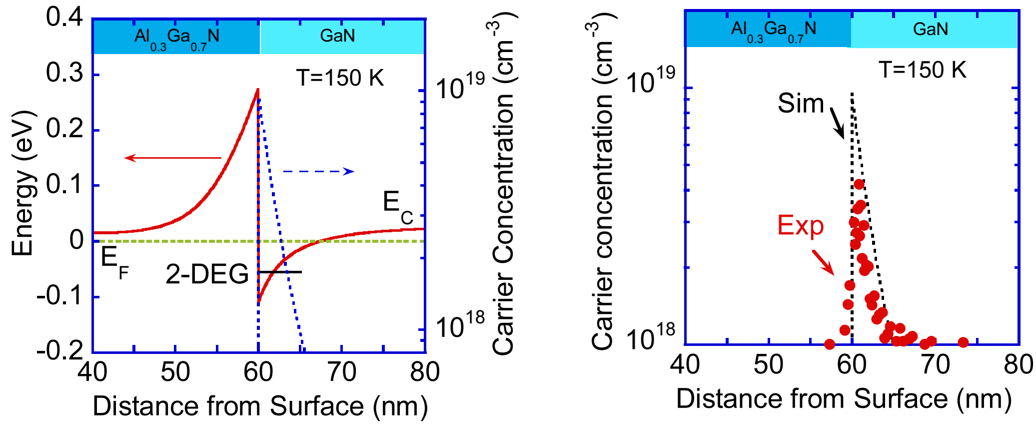

Fig. 4 Left side: Band diagram and the carrier concentration distribution of the $Al_{0.3}Ga_{0.7}N$/GaN heterojunction vs. distance from the surface. Right side: Experimental (full circles) and simulated (dotted line) carrier concentration vs. the distance from the surface. The experimental data were calculated from a CV measurement done at 150 K.

A well established method to analyze heterostructures are CV measurements. With this method the depth distribution of the carrier concentration can be measured. In the right side of Fig. 4 the carrier concentration of an $Al_{0.3}Ga_{0.7}N$/GaN heterojunction measured by CV is potted versus depth (full circles) together with the simulated electron profile (dotted line). The CV measurement was performed at 150 K. The depth position (~ 60 nm) and the maximum electron concentration of about $4x10^{18}$ cm^{-3} are in excellent agreement with the simulated profile. From the width of the electron distribution and the peak electron concentration a sheet carrier concentration of about $1.6x10^{12}$ cm^{-2} is estimated. Hall effect measurements were not possible due to the high conductivity of the 3C-SiC substrates.

4 Conclusion

We successfully fabricated cubic $Al_xGa_{1-x}N$/GaN heterostructures by MBE on 3C-SiC (001) substrates. An additional luminescence band at 3.250 eV was observed at low temperature which we attribute to a 2-DEG transition. Intensity dependent and voltage dependent PL measurements showed characteristic shifts of this transition of 4.5 meV/decade and 1.3 meV/V, respectively, due to the change in the carrier confinement by varying the laser excitation power or the external bias voltage, respectively. These shifts are quantitatively verified by a self consistent solution of the Schrödinger and Poisson equation. CV measurements at T = 150 K reveal a clear evidence for the existence of a 2-DEG, and a sheet carrier concentration of about $1.6x10^{12}$ cm^{-2} is measured at the interface in good agreement with the numerical simulation.

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