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Capacitance properties and simulation of the AlGaN/GaN Schottky heterostructure

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ABSTRACT

The paper presents the results of capacitance measurements on GaN/AlGaN/GaN Schottky heterostructures grown on an Al_2O_3 substrate by Low-Pressure Metal–Organic Vapour-Phase Epitaxy (LP-MOVPE). Dependences of the capacitance–voltage (CV) characteristics on the frequency of the measuring signal allow analysing the properties of the 2D electron gas (2DEG) at the AlGaN/GaN heterojunction. Exact location of the hetero-interface below the surface (20 nm) was determined from the concentration profile. Temperature variations of the CV curves reveal the influence of bulk defects in GaN and of the traps at the AlGaN/GaN interface. Electrical activity of these defects was characterized by capacitance Deep Level Transient Fourier Spectroscopy (DLTFS). Experimental results of CV measurements were supported by simulating the properties of the GaN/$Al_{0.2}GaN_{0.8}$/GaN Schottky heterostructure in dependence on the influence of the concentration of donor-like traps in GaN and of the temperature upon the CV curves.

1. Introduction

Novel quantum-coupled electron devices based on heterostructures impose high demands upon the quality of production. Recently, the most significant progress in HEMT technology has been made on the wide band-gap semiconductor GaN intended mainly for power and high-frequency applications [1].

Along with the progress in these devices and structures it is inevitable to improve and/or develop also diagnostic methods. The most often analytical methods include the capacitance techniques based on the spreading of the space charge region (SCR). From the practical point of view it is appropriate to use a Schottky contact for analysis of some electro-physical properties of the AlGaN/GaN heterostructure. The voltage dependence of capacitance (CV) allows revealing the depth profile of free charge carriers and the position of the quantum well (QW). From the CV curve one can simply calculate also the density of the two-dimensional electron gas (2DEG) [2].

In the design of AlGaN/GaN HEMTs it is difficult to avoid large gate leakage currents and the drain current collapse. These phenomena are closely related to the density and energy distribution of the traps at the AlGaN/GaN interface and with the electrical activity of deep defects in the active region of the heterojunction [3]. Deep level transient spectroscopy (DLTS) is one of the most powerful techniques for characterizing deep level defects in semiconductors. It provides all important defect parameters, such as the thermal activation energy (E_T), electron and hole capture cross sections ($\sigma_{n,p}$) and defect concentration (N_T). DLTS is often used to characterize the quality of the GaN substrate [4].

In this paper, CV characteristics of NiAu/GaN/AlGaN/GaN Schottky diodes measured at various temperatures in the range from 80 to 500 K are analyzed. CV measurements at a frequency of 1 MHz allowed us to obtain the concentration profile using a simple model [2]. Capacitance measurements were completed by frequency dependences. To verify the CV measurements, a model was used simulating the capacitance properties of the Schottky contact with a quantum well. The influence of deep energy levels upon the shape of CV curves was interpreted by Deep Level Transient Fourier Spectroscopy (DLTFS) measurements.

2. Sample preparation

The GaN/AlGaN/GaN Schottky structures used in this study were grown by LP-MOVPE on a sapphire substrate. The layer structure consisted of a 2 μm thick GaN buffer followed by a 20 nm thick $Al_{0.2}Ga_{0.8}N$ barrier layer and a 5 nm thick GaN cap layer

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Ti / Al / Ni / Au (20/100/40/50 nm)		Ni / Au (40/130 nm)
UN GaN	cap layer	5 nm
$Al_{0.2}Ga_{0.8}N$	barrier layer	20 nm
GaN:Fe	buffer	2 μm
Al_2O_3	substrate	

Fig. 1. Schematic description of the GaN/AlGaN/GaN Schottky structure on a sapphire substrate.

on top (Fig. 1). Ohmic contacts were prepared by evaporation of a Ti (20 nm)/Al (100 nm)/Ni (40 nm)/Au (50 nm) multilayer and rapid-thermal annealing at 850 °C in N_2 atmosphere for 35 s. Next, mesa insulation (~100 nm) was formed by reactive ion etching AlGaN/GaN in CCl_4 gas plasma. For the gate contact, a nickel (40 nm) layer covered by a gold (130 nm) layer were patterned by electron beam lithography to get different Schottky contact areas (100 μm × 100 μm and 200 μm × 200 μm). Finally, rapid thermal annealing in N_2 at 430 °C was performed. CV measurements on a series of samples allowed to retrieve the Schottky barrier height between 0.68 and 0.71 eV.

3. Simulations

The model was employed to simulate metal/GaN/Al_xGaN_{1-x}/GaN Schottky heterostructures with concentration of aluminium $x = 0.2$ and with a Schottky barrier height $\phi_b = 0.7$ eV. In simulations using the trap-assisted-tunnelling (TAT) model [5,6] we considered the Huang–Rhys factor $S = 6.5$ and effective phonon energy $\hbar\omega_0 = 0.066$ eV. The concentration of traps was assumed to be $N_t = 2 \times 10^{17}$ cm^{-3}. The distribution function of the traps in the forbidden band forms a band of traps at energy level $E_C - E_T = 0.5$ eV from the conduction band edge. The overall charge Q_{het1} at the upper (GaN/AlGaN) junction is negative, Q_{het2} at the lower (AlGaN/GaN) junction is positive and the value of the charge is a material parameter depending on the molar concentration of aluminium. In the case of $Al_{0.2}Ga_{0.8}N$ one has $Q_{het1,2} = \mp 2.16 \times 10^{-6}$ (As/cm^2), band offsets $\Delta E_C = 0.419$ eV and $\Delta E_V = 0.084$ eV. The permittivity ratio is $\varepsilon_{rAlGaN}/\varepsilon_{rGaN} = 0.975$.

The band diagram and the concentration profile of the structure are shown in Figs. 2 and 3.

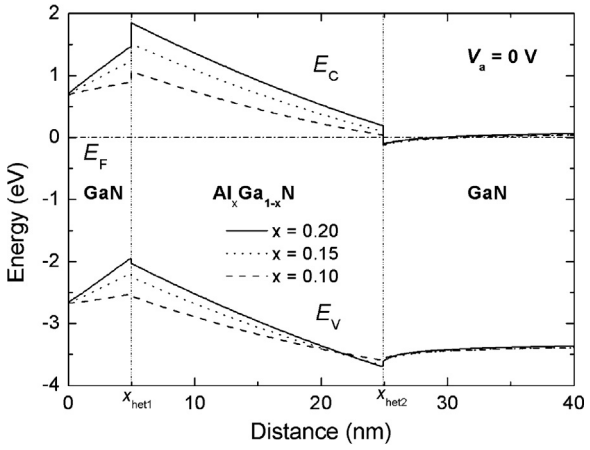

Fig. 2. Band diagram of the metal/GaN/AlGaN/GaN Schottky heterostructures under thermodynamic equilibrium for various concentrations of aluminium.

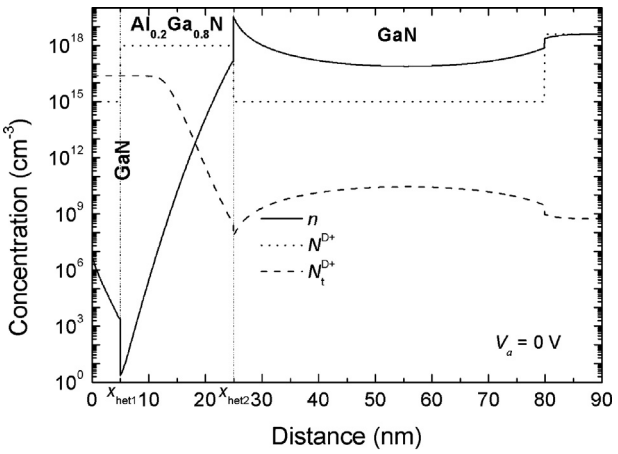

Fig. 3. Concentration profile of the metal/GaN/AlGaN/GaN Schottky heterostructure under thermo-dynamic equilibrium for molar concentration of aluminium $x = 0.2$.

The capacitance model of the GaN/AlGaN/GaN Schottky structure was prepared using the structure editor MDRAW tool from the Synopsys TCAD package [7]. For structures with quantum wells (QW) a very dense mesh is typical. In the QW region the mesh spacing must be at least 10 to 100 times smaller than the QW width to ensure good convergence of the numerical electro-physical solver [8]. Electro-physical behaviour of the structure was studied using the simulation tool SDEVICE [7]. For simulations the hydrodynamic mode (HD) was used and since very strong and inhomogeneous fields are typical for HEMT operation, the high-field effects upon the electron transport have to be taken into account. Moreover, the Fermi-Dirac statistics must be turned on instead of the default Boltzmann statistics. If deep level traps and interface charges are considered in simulations, the HD model must be used, which is also crucial for non-isothermal, AC coupled and transient simulations. Simulations of CV curves for several concentrations of traps in GaN (Fig. 4) and temperatures (Fig. 5) were performed. For these simulations a single electron-like deep energy level with activation energy $E_T = 0.5$ eV with respect to the conduction band was taken into account. From simulations it is clear that temperature has a dominant effect on the slope of the CV curves. However, for voltages close to the pinch-off voltage direct tunnelling and trap-assisted tunnelling processes become more significant. However, consideration of these processes (especially trap-assisted tunnelling) in the

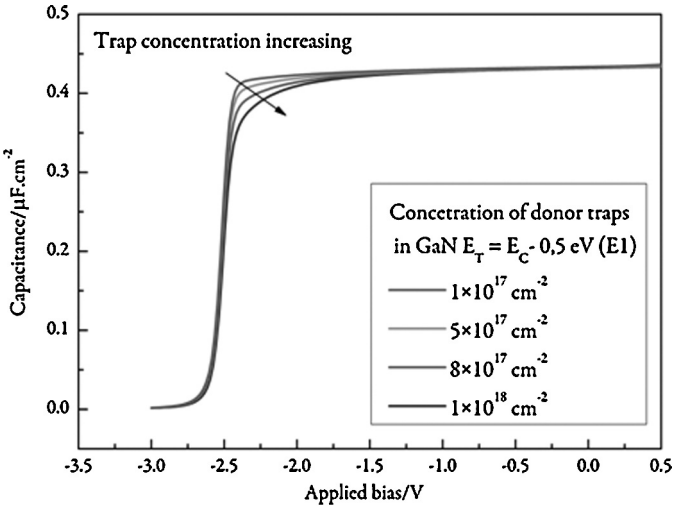

Fig. 4. Simulations of the influence of the concentration of electron-like traps in GaN.

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