Published in : Journal of Crystal Growth (2001), vol. 230, pp. 596-601.
Authors : N. D. Nguyen, M. Germain, M. Schmeits, R. Evrard, B. Schineller, M. Heuken
Status : Postprint (Author's version)

Experimental and theoretical investigations of the electrical properties of undoped and magnesium-doped GaN layers

N.D. Nguyen[a], M. Germain[a], M. Schmeits[a], R. Evrard[a], B. Schineller[b,c], M. Heuken[b,c]

[a]*Institut de Physique, Université de Liège, B5, 4000 Liège, Belgium*

[b]*Institut für Halbleitertechnik, RWTH Aachen, Temp1ergraben 55, D-52056 Aachen, Germany*

[c]*AIXTRON AG, Kackertstr. 15-17, D-52072 Aachen, Germany*

ABSTRACT

The ac characteristics of GaN : Mg and undoped GaN layers, grown by MOVPE on sapphire substrates, are measured for a wide range of temperature and bias conditions, in order to investigate the effect of the magnesium-related level on the transport properties. Two peaks, whose height and position depend on the measurement temperature, are observed in the admittance curves (G/ω versus frequency) of the Mg-doped samples, whereas only one peak appears in undoped samples. The study of the frequency dependence of the impedance, with a model including the two metallic Au/GaN junctions, the GaN layer itself, shows that, besides the effect of the differential resistance of the layer which plays a role in both sample types, the presence of a Mg-related deep level contributes to the observed variations of the peaks in the admittance curves of the p-doped samples. Results of a theoretical steady-state and small-signal analysis based on numerical modelling of the Au/GaN/Au heterostructure complete our analysis.

Keywords : A1. Characterization ; A1. Defects ; A3. Metalorganic vapor phase epitaxy ; B1. Nitrides ; B2. Semiconducting gallium compounds ; B3. Schottky diodes

PACS : 84.37.+q; 73.61.Ey; 71.55.Eq; 73.40.Sx

1. Introduction

Research on GaN attracts considerable interest since the nitride-related materials lead to numerous blue and ultra-violet (UV) optoelectronic devices, as well as to applications in high-power and high-frequency electronics [1]. To improve the performances of these components, the understanding of the transport mechanisms in the GaN-based structures, including the role of the doping impurities, is thus strongly demanded. Mg is known to be a p-type dopant of GaN [2]; its influence on the electrical transport through GaN layers is, however, not yet completely understood. In particular, the electrical activation energy of the Mg-related level lies in a wide range according to different authors throughout literature, i.e. between 120 and 300 meV [3,4]. This value, larger than the usual ionization energy of dopants, leads to a behaviour where Mg acts both as dopant and deep impurity. Admittance-versus-frequency measurements in addition to capacitance-versus-voltage measurements are particularly well-suited experiments for the characterization of such a deep level. We have thus measured the ac electrical properties of undoped and Mg-doped GaN layers at different temperatures. We perform a detailed analysis of the resulting electrical characteristics for different bias voltages. We analyze the role of the contacts, of the GaN film and the possible effect of the sapphire substrate. Indeed, the GaN crystals are grown on sapphire substrate, which can affect the electrical characteristics. The contacts are of Schottky type and the whole structure can be represented by an equivalent circuit including two back-to-back Schottky diodes and a series resistance due to the contribution of the GaN layer. Finally, by comparing the experimental results to numerical simulations of the system, we show the effect of the Mg doping impurity on the electrical characteristics and its influence on the conduction mechanisms.

2. Experiments

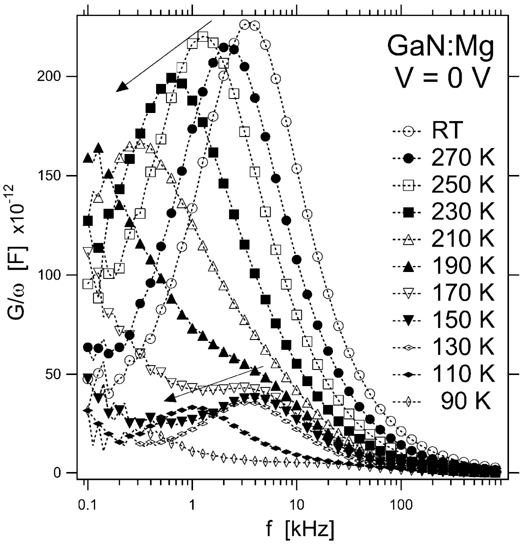
The GaN layers, grown by MOVPE, consist of a nucleation (low temperature buffer) layer directly on top of the sapphire substrate, followed by an undoped GaN layer either followed or not followed by a GaN : Mg layer. For Mg-doped layers, the $Cp_2Mg/TEGa$ gas phase ratio, which determines the amount of Mg atoms incorporated into the layer, is around 0.1% and the deposition temperature lies in the neighbourhood of 1100°C. The thickness of the layers in undoped samples is 2 µm. In the case of doped samples, the GaN : Mg layer is 2 µm thick while the buffer layer is of the order of 1-2 µm. Metallic contacts were evaporated on the top of the GaN layers consisting of 150nm Au for undoped samples and l0nm Ni/120 nm Au for p-type samples. The contacts have a diameter of 0.5 and 1 mm, respectively for Mg-doped and undoped layers and are 2 mm apart from each other in both types. They are not annealed.

Impedance and admittance ac measurements were performed using a Hewlett-Packard 4192A LF impedance analyzer, for frequencies in the range of 100 Hz-1 MHz and for bias voltages ranging from -3 to +3V. The oscillation level was equal to 0.05 V. The temperature was varied down to 80K, with a precision of 0.02K. The measurements were performed between two co-planar contacts on the GaN surface.

3. Experimental results

We first discuss the electrical properties under ac conditions of a typical Mg-doped sample. We plot in Fig. 1, G/ω, where G is the conductance and $\omega = 2\pi f$, versus the frequency for different temperatures. The bias voltage is equal to 0V. At room temperature (293 K), the G/ω curve presents a large peak at 4 kHz. As the temperature is lowered, this peak shifts to lower frequencies and its amplitude decreases. At 190 K, a second peak, with a smaller amplitude appears at 5 kHz, which also seems to move to the low-frequency region as the temperature decreases down to 90K. The frequency dependence of the admittance is also noticeable in the capacitance-versus-frequency curves (not shown here). One can distinguish two parts in the curves : the low-frequency capacitance, which varies with the bias voltage, is separated from the high-frequency regime by a cut-off frequency at 4 kHz. The capacitance at high frequency, 0.4 pF, is relatively small and does not vary with the bias voltage.

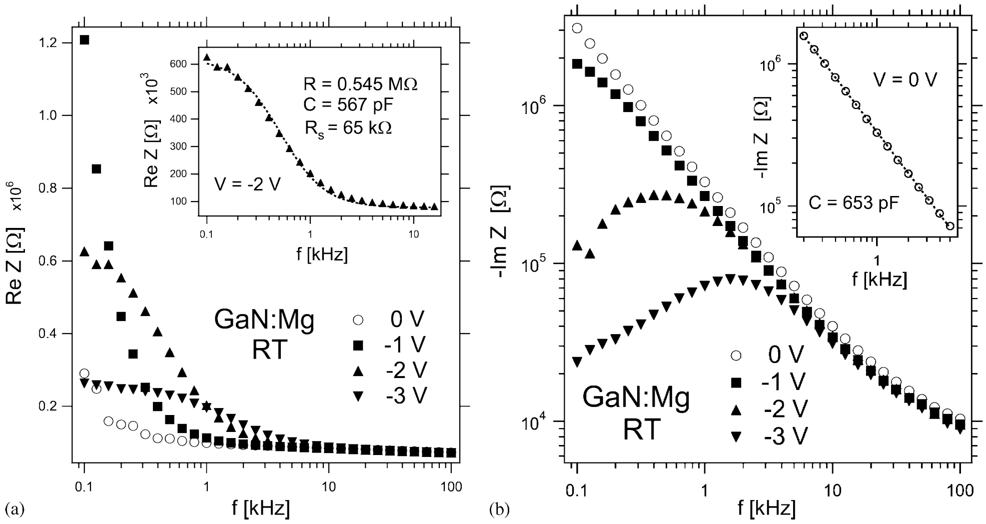
Fig. 1. *G/ω-versus-frequency at different temperatures and zero bias voltage for a Au/GaN : Mg/Au structure. Dashed lines are shown for visual convenience. Arrows show the observed shifts of both peaks as the temperature is decreased.*



Let us first discuss the behaviour of the system at room temperature. The existence of a cut-off frequency in capacitance curves of such shape, associated with the presence of a peak in the frequency dependence of G/ω, is usually related to the presence of a deep level in the layer [5]. At low frequencies, deep states, which are involved in transitions with either the valence or the conduction band, follow the modulation of the applied voltage, yielding the plateau regime in the capacitance. At intermediate frequencies, their response is progressively reduced and beyond a given frequency (which would be equal to 4 kHz in our case), none of the defect states is able to follow the small-signal voltage. The value of the capacitance is then related to the concentration of residual impurities as well as to the deep level concentration. As Mg gives rise to a relatively deep level in the band gap of GaN, it could be responsible for the appearance of the peak in G/ω-versus-frequency measurement. However, the system under study is more complicated than a single Schottky barrier. On the one hand, the high resistance of the layer itself can be responsible for the peak in the admittance curves. On the other hand, we must not forget that the measurements are performed between two coplanar contacts on the top of the GaN layer. Thus, the measured capacitance results from the presence of two contacts in series. These two contacts behave like two Schottky barriers back-to-back: when one is forward biased, the other is reverse biased. The study of this kind of system has been performed in detail by our group for Au/ZnSe/GaAs hetero-structures [6]. It can be shown that the presence of two diodes in series can be modelled by two RC circuits in series: each RC representing, in our case, one of the Au/GaN junctions. This equivalent circuit network also leads to the presence of a cut-off in the C-f curves, when the capacitances are not exactly equal [7]. At high frequency, the two capacitances of the contacts in series dominate; at low frequency, their differential resistance cannot be ignored and plays a role in the value of the equivalent capacitance.

In the analysis of the electrical characteristics of such a structure, the study of the real and imaginary parts of the impedance at different bias voltages turns out to be especially useful. Indeed, as the two junctions appear in series, the electrical characteristics of both junctions simply add in the impedance curves. Figs. 2(a) and (b) show, respectively, the real and imaginary parts of the impedance plotted against frequency in logarithmic scales, for different values of the bias voltage, at room temperature. At zero bias, the imaginary part of the impedance, -Im(Z), is well-fitted by a ω^{-1}-like decreasing behaviour in logarithmic scale, typical of a single capacitance. The result of the fit is shown in the inset of Fig. 2(b). As the bias voltage increases in amplitude, this equivalent capacitance decreases and for bias voltages higher, in absolute values, than 1V, a peak appears in the Im(Z)-f curve. The Im(Z)-f characteristics can then be modelled by a circuit with a resistance R in parallel with a capacitance C. The inset of Fig. 2(a) shows the result of the fit on Re(Z) with this model at a bias voltage of -2 V. The Re(Z)-f characteristics reveal moreover the presence of an additional resistance in series, named R_S. It corresponds to the GaN layer between the two depletion layers of the contacts. The obtained value of this resistance in series is equal, at room temperature, to 65 kΩ. The behaviour of the system can thus be understood as following : at low bias voltages, the bias applies on both contacts; the differential resistances of these contacts are so high that the behaviour of the contacts under small-signal conditions is dominated by their capacitance. Thus, the capacitance deduced from the slope of -Im(Z)-f in logarithmic scale corresponds to the equivalent capacitance of the two contacts in series. On the contrary, for high bias voltages, one of the contacts is reverse biased whereas the other one is forward biased. Consequently, the voltage is mainly applied to the reverse-biased junction and the ac equivalent circuit of our structure is a single RC parallel circuit correspond ing to the reverse-biased junction, to which one should add the resistance of the layer itself, R_S. The capacitance of the forward-biased junction is so high that it is not observable in the impedance curves.

***Fig. 2**. Real (a) and imaginary (b) part of impedance Z versus frequency at different bias voltages and room temperature for a Au/GaN: Mg/Au structure. Inset of (a): experimental result for bias voltage of -2 V and related fit (dashed line). Inset of (b): experimental result for null bias and related fit (dashed line). The insets are shown with values of the fits. See text for details.*



From this analysis, we can already deduce an estimation of the concentration of the electrically active doping impurities, which could not be obtained from the C-V curves of the complete structure [7]. We use the values of the capacitance obtained from the fits of -Im(Z) at bias voltages sufficiently high in amplitude (higher than 1.5 V) so that only the reverse-biased junction contributes to the electrical properties. We can then assume that the voltage is mainly applied to this reverse-biased junction and determine a rough estimation of the concentration of electrically active impurities, using the conventional $1/C^2$-V analysis. This gives a first estimation of the electrically active impurity concentration of about 4×10^{18}cm^{-3}. This value should, however, be taken with caution: a modulation of the applied voltage results in a variation of the hole population in the valence band which is due the modulated occupancy level of all acceptor impurities, including deep and possibly residual shallow dopants.

At low bias voltage, the system behaves like a single equivalent capacitance corresponding to the two capacitances of the contacts in series, plus the resistance of the layer itself. The position of the main peak in the G/ω-versus-frequency curve at room temperature can be related to the cut-off frequency of an RC series circuit which is given here by $(2\pi R_S C_{tot})^{-1}$, where C_{tot} is the total equivalent capacitance of the two junctions, including the contributions of deep impurities, and R_S is given by the high-frequency regime of the real part of the impedance. The variation of this peak with temperature is not only due to the temperature dependence of R_S but also of the defect capacitances [5].

The second peak which appears in the *G*/*ω* versus-frequency curves, at temperatures lower than 150 K, is weakly dependent on the temperature in the range of 150-130K, then moves moderately to lower frequencies when the temperature is further decreased. We note that it does not vary with the bias voltage. In our measurements, only one peak is appearing in the ac characteristics of the undoped samples. Fig. 3 shows the admittance curves of an undoped sample for null bias voltage, with the temperature ranging from room temperature (293K) to 90K. Again, a large peak is present at room temperature, which can easily be understood by the cut-off frequency resulting from the equivalent capacitance of both junctions in series, themselves being in series with the differential resistance of the layer. This is confirmed by the analysis of the real and imaginary part of the impedance at different bias voltages, similar to the one performed for doped samples above. Here, the series resistance of the layer is smaller than that for the Mg-doped samples, which leads to a higher cut-off frequency. Moreover, one sees that, in the case of doped samples, both the position and the amplitude of the peak in *G*/*ω* vary with the temperature (see Fig. 1) whereas in the case of undoped sample, only the position of the peak changes with temperature, its height being unchanged. To complete our analysis, we have performed a theoretical small-signal analysis based on numerical modelling [8] of the Au/GaN/Au heterostruc-ture, including the presence of the Mg deep level. Fig. 4(a) shows the energy band diagram of this system. Fig. 4(b) displays the small-signal variation of the concentration of electrons trapped on the Mg level as well as the hole concentration in the layer. The Mg level is shown to be deep enough to cross the Fermi level at room temperature. This implies that, under ac conditions, both the hole concentration at the edge of the depletion layer and the electron concentration on the deep level are modulated and contribute to the capacitance of the Au/GaN junction in Mg-doped samples. As a consequence, the capacitance of the Schottky contact varies with the temperature, whereas in undoped samples, where no deep level is present, the capacitance of the contact is temperature independent. As the height of the peak in *G*/*ω* essentially varies as *C*/2, the comparison between Figs. 1 and 3 confirms that a deep level is present in doped samples, which may possibly be related to magnesium.

Fig. 3. *G/ω-versus-frequency at null bias and different temperatures for a Au/GaN/Au structure based on an undoped GaN sample. Dashed lines are shown for visual convenience.*

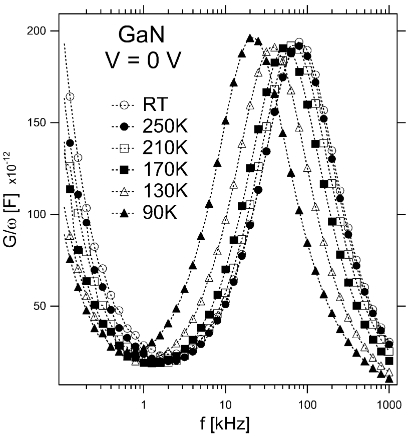
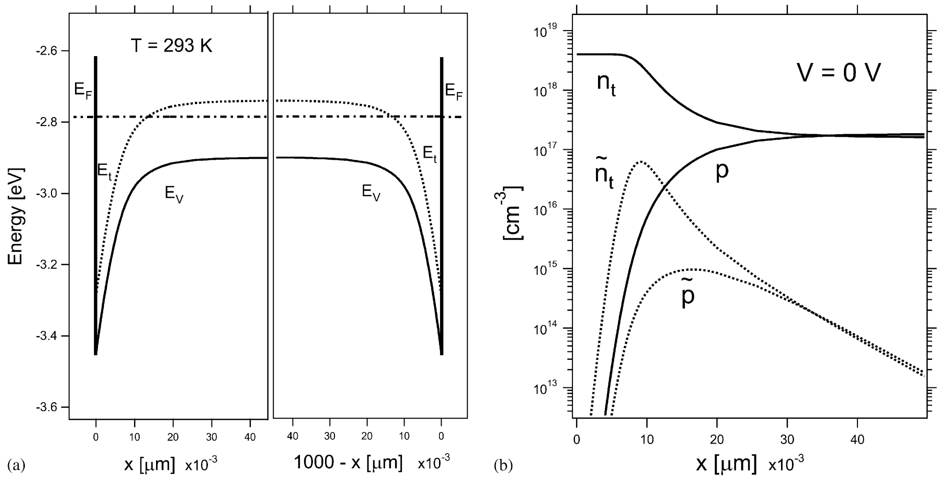


Fig. 4. *(a) Band diagram for a double metal-GaN structure at room temperature and zero applied voltage. The valence band edge* E_V *as a function of the x-coordinate is plotted with a defect level* E_t *at 160meV from* E_V*. The Fermi level* E_F *in the bulk lies between* E_t *and* E_V*. The doping level for the deep defect is taken as* $N_t = 4 \times 10^{18}$ cm^{-3}*. The Schottky barrier height is taken as 0.67 eV. (b) Steady-state and absolute value of small-signal ac component (at frequency of 100 Hz) at zero bias for hole concentration p and concentration of occupied states* n_t *for the left Au/GaN junction.*



4. Conclusions

The analysis based on equivalent electrical circuit models for Au/GaN/Au junctions is used to separate the contribution of defect states from junction effects in capacitance and conductance response curves. For this purpose, impedance and admittance measurements were performed and allowed the elaboration of a model that can explain such a behaviour of the system under various conditions of biasing and temperature. The main peak in the (G/ω)-versus-frequency curves is attributed to the presence of the capacitance of both junctions in series with the resistance of the layer. This capacitance of the contacts has contributions from both the modulated occupancy level and depletion layer edge. Further measurements and numerical simulations will give a complete analysis of the observed phenomenon.

Financial support by an INTAS grant N 97-0995 and by the Belgian Fonds National de la Recherche Scientifique (contract 9.4565.96F) are gratefully acknowledged.

References

[1] J.-Y. Duboz, Phys. Stat. Solidi (A) 176 (1999) 5.

[2] S. Nakamura, in: B. Kramer (Ed.), Advances in Solid State Physics 38, Vieweg, Braunschweig/Wiesbaden, 1999 p. 1.

[3] S.C. Jain, M. Willander, J. Narayan, R. Van Overstraeten, J. Appl. Phys. 87 (2000) 965

[4] J.W. Huang, T.F. Kuech, H. Lu, I. Bhat, Appl. Phys. Lett. 68 (1996) 2392.

[5] W.G. Oldham, S.S. Naik, Solid-State Electron. 15 (1972) 1085.

[6] R. Martinez, M. Schmeits, R. Evrard, Adv. Mater. Optics Electron. 3 (1994)81.

[7] M. Germain, R. Evrard, S. Lampe, M. Heuken, J. Electron. Mater. 27 (1998) 29.

[8] M. Sakhaf, M. Schmeits, J. Appl. Phys. 80 (1996) 6839.