

Quantum Effects in Metal-Oxide Interfaces

Dr. Sofia Rodriguez, Dr. Julian Styles

University of Cambridge, UK

Abstract—The current-voltage (I - V) characteristics of Pd/n-GaN Schottky barrier were studied at temperatures over room temperature (300-470K). The values of ideality factor (n), zero-bias barrier height

(b_0), flat barrier height (b_F) and series resistance (R_s) obtained from I - V - T measurements were found to be strongly temperature dependent while (b_0) increase, (n), (b_F) and (R_s) decrease with increasing temperature. The apparent Richardson constant was found to be $2.1 \times 10^{-9} \text{ Acm}^{-2}\text{K}^{-2}$ and mean barrier height of 0.19 eV. After barrier height inhomogeneities correction, by assuming a Gaussian distribution (GD) of the barrier heights, the Richardson constant and the mean barrier height were obtained as $23 \text{ Acm}^{-2}\text{K}^{-2}$ and 1.78eV, respectively. The corrected Richardson constant was very close to theoretical value of $26 \text{ Acm}^{-2}\text{K}^{-2}$.

Keywords—Electrical properties, Gaussian distribution, Pd-GaN Schottky diodes, thermionic emission.

I. INTRODUCTION

GALLIUM NITRIDE (GaN) has a direct band gap of 3.4 eV, which has a broad range of electrical applications, especially in high temperature electronic devices, optoelectronic and high-power devices. Intensive activities on high-power devices, short-wavelength light (blue, violet) emitting diodes (LEDs), and laser diodes (LDs) have been conducted [1].

To construct such devices, it is necessary first to clarify the physics of metal/GaN interface and its influence on electrical characteristics of metal/GaN Schottky diodes. Many researchers using high work function metals as Schottky contacts like Ni, Pt and Pd report Schottky contacts on GaN [2]-[9]. It is well known that the electrical characteristics of a Schottky contact are controlled mainly by its interface properties. Thus, the study of interface states is important for the understanding of the electrical properties of Schottky contacts.

The analysis of the I - V characteristics of metal/semiconductor diodes at wide temperature range allows us to understand different aspects of barrier formation and current-transport mechanisms and gives information about the quality of the contacts especially at temperatures higher than room temperature. A lot of work has already been reported on electrical characterization but there are few works studied the

M. R. Hashim is with Nano-Optoelectronics Research Laboratory, School of Physics, Universiti Sains Malaysia, 11800-Penang, Malaysia.

temperature dependence of electrical characteristics of GaN Schottky diodes [10]-[14]. Akkal *et al.* [10] investigated the current-voltage characteristics of Au/n-GaN Schottky diodes

below room temperature in the range 80-300 K. Osvald *et al.* [11] investigated the temperature dependence of the electrical characteristics of GaN Schottky diodes with two crystal polarities (Ga- and N-face). They reported a decrease in the barrier height with a decrease in temperature and an increase in ideality factor for both polarities. Arehart *et al.* [12] studied the impact of threading dislocation density on the Ni/n-GaN Schottky diode using forward measurements. Tekeli *et al.* [13] investigated the behavior of the forward bias (I - V - T) characteristics of inhomogeneous (Ni/Au)- $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}/\text{AlN}/\text{GaN}$ heterostructures in the temperature range of 295-415 K using double layers of metal and multi layers of GaN and AlN. Recently, Ravinandan *et al.* [14] reported on the temperature dependent electrical characteristics of the Au/Pd/n-GaN Schottky diode in the temperature range of 90-410 K.

This study aims to gain insight about the current-transport mechanism through a single metal contact of palladium on GaN (Pd/GaN) by measuring their electrical properties from room temperature to well above it (300-470 K). This is very important in order to get more accurate results on single metal Schottky contact on single GaN layer operating at higher temperature. The values of ideality factor (n), zero-bias barrier height (b_0), flat barrier height (b_F) and series resistance (R_s) were extracted from the forward bias I - V measurements. The temperature dependence of the Schottky barrier height of Pd/GaN are interpreted based on the existence of the Gaussian distribution (GD) of the barrier heights around a mean value due to the barrier height inhomogeneities prevailing at the metal-semiconductor interface.

II. EXPERIMENTAL PROCEDURES

The samples used in this study were commercial n-GaN grown by metalorganic chemical vapor deposition (MOCVD) on Al_2O_3 substrates. The electron concentration (Si doped) obtained by Hall measurements was $n = 1 \times 10^{17} \text{ cm}^{-3}$. The samples were cleaned first with acetone and methanol, then secondly in 1:20 $\text{NH}_4\text{OH}:\text{H}_2\text{O}$ for 10 min, followed by a third cleaning in 1:50 $\text{HF}:\text{H}_2\text{O}$ solution to remove the surface oxides. This was followed by a fourth cleaning in 3:1 $\text{HCl}:\text{HNO}_3$ at 80 °C for 10 min. Between the cleaning steps, the samples were rinsed in deionized water. After cleaning the diode was completed by deposition of Pd on a portion of the sample of n-GaN using the A500 Edwards RF magnetron sputtering unit. The ultimate pressure was 1×10^{-6} mbar, which was raised to 2×10^{-2} mbar by purging the chamber with high purity argon gas (Ar 99.99%); the power of sputtering was 150W. The (I - V) measurement of the sample was carried out using the Keithley model 2400 on different temperature in the range of 300-470K and in the dark. The operation temperature of the diode was measured by a calibrated K-type thermocouple mounted on the device.

III. RESULTS AND DISCUSSION

Typical current-voltage (I - V) characteristics of the Pd/GaN Schottky diode measured in atmospheric conditions, in the temperature range of 300-470K are shown in Fig. 1. From the figure, one can observe that the contact of Pd with an n-type GaN acts as rectifying junction for forward and reverse currents. The figure also shows an increment of the linear region as the temperature increases. Meanwhile the non-linear region shows a decrease of series resistance as temperature increases (Fig. 1 (b)).

Current transports in a diode are governed by two regimes. At low voltage, it is governed by thermionic emission and at higher voltage it is governed by other mechanisms than thermionic emission [10].

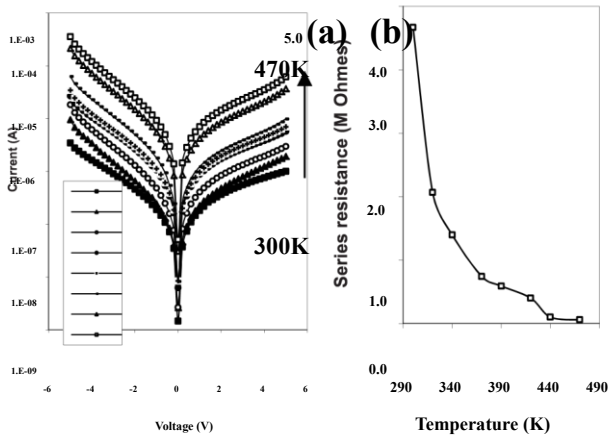


Fig. 1 Temperature dependent I - V plot (a) and the variation of series resistance (b) for the Pd/GaN Schottky diode in the temperature range (300–470K)

The forward I - V characteristics were analyzed using standard thermionic emission relation for electron transport from a metal-semiconductor with low doping concentration. It is given by the following equation for $V > 3kT/q$ [15]-[17]

$$I = I_0 \exp \left(\frac{qV}{nkT} - \frac{V}{R_S} \right) \quad (1)$$

where V is the voltage across the diode, n the ideality factor, k is the Boltzman constant, R_S is the series resistance and I_0 is the saturation current given by

$$I_0 = A A^{**} T^2 \exp \left(-\frac{q\Phi_{B0}}{kT} \right) \quad (2)$$

where q is the electron charge, T is the temperature in Kelvin, A is the contact area, A^{**} is the Richardson constant and Φ_{B0} is the Schottky barrier height. By plotting $\ln(I)$ vs. V for each temperature in the range (300-470K) for the Pd/GaN Schottky diode we get a straight line with the slope $= q/nkT$ and yintercept ($V=0$) at $\ln I_0$. From the value of I_0 , Schottky barrier height Φ_{B0} (zero-bias barrier height) was calculated using (2) [18]. In addition, from the slope the ideality factor n was calculated, which is a measure of the thermionic emission current transport ideality. Fig. 2 shows the barrier height and ideality factor as a function of temperature in the temperature range (300–470K) for the Pd/GaN Schottky diode.

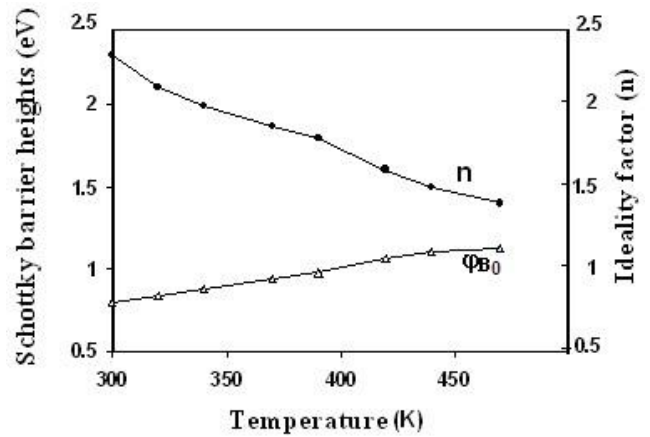


Fig. 2 Barrier height and ideality factor as a function of temperature in the temperature range (300–470K) for the Pd/GaN Schottky diode

From this figure, one can observe that the ideality factor n decreases with increasing temperature while the zero-bias barrier height increased with increasing temperature, which agrees with the thermionic emission theory. These indicate that the contact between Pd and GaN enhanced with increasing temperature.

When ideality factor is larger than unity thermionic emission is not the only mechanism that contributes to the transfer of current. The barrier height obtained under the flat band condition is called the flat band barrier height and is considered as the real fundamental quantity. The flat band barrier height, Φ_{BF} can be derived from Φ_{B0} using the following equation [11]:

$$\Phi_{BF} = \Phi_{B0} - (n-1)(E_C - E_F) \quad (3)$$

where E_F is the Fermi energy and E_C is the conduction band energy, the energy difference between the conduction band and the Fermi level is given by

$$E_C - E_F = \frac{q\Phi_{BF}}{n} = \frac{q\Phi_{B0}}{n} - \frac{q(N_D - N_A)}{4N_D} \quad (4)$$

where N_C is the effective density of states in the conduction band and N_D is the donor concentration. Assuming that the electron effective mass and N_D do not change with the temperature, but the effective density of states in the conduction band N_C will change with the temperature according to the relation N_C (cm⁻³) = $2.6 \times 10^{18} (T/300)^{3/2}$ [10], [19]-[21]. Based on these equations the flat band barrier height Φ_{BF} can be obtained. The results are shown in Fig. 3. One can observe that the flat barrier height slightly decreased with temperature, while the zero-bias barrier height increases with temperature. The difference between the zero-bias and the flat barrier height values may come from the fact that, the thermionic emission is not the only mechanism by which electrons can cross the Schottky barrier.

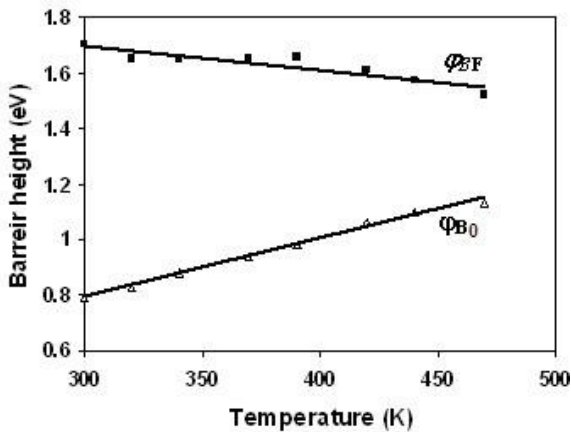


Fig. 3 The barrier height for Pd/n-GaN Schottky diodes vs. temperature

Equation (2) can also be used to construct a Richardson plot of $\ln(I_0/AT^2)$ versus $1/kT$, with the slope giving Φ_{B0} and A^{**} is determined by the intercept. This plot is shown in Fig. 4.

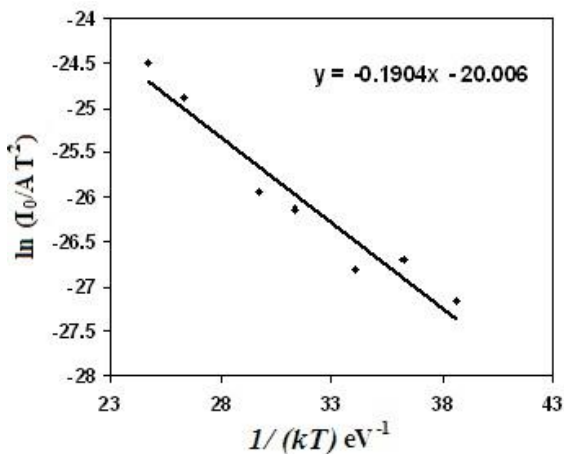


Fig. 4 Richardson plot, $\ln(I_0/AT^2)$ versus $1/(kT)$ for the Pd/GaN in the temperature range (300–470K) for the Pd/GaN Schottky diode

From the figure, Richardson constant and zero-bias Schottky barrier values were $2.1 \times 10^{-9} \text{ Acm}^{-2}\text{K}^{-2}$ and 0.19 eV respectively. The value of Richardson constant is much lower than the known

theoretical value of $26 \text{ Acm}^{-2}\text{K}^{-2}$ for n-GaN. The deviation in A^{**} is generally explained by the barrier inhomogeneity of the contact, which means that it consists of high and low barrier areas at the interface mainly due to the formation of different oxides layer thickness between the metal and semiconductor. In addition, the effective area for current conduction (A_{eff}) is significantly lower than the geometric contact area (A_{geom}) due to preferential current flow through lower barrier height regions [22], [23].

In order to explain the abnormal behavior between the theoretical and experimental values of Richardson constant A^{**} , let us assume that the distribution of the barrier heights is a Gaussian distribution (GD) with a mean value Φ_B and standard deviation σ_s , which can be given by [24]-[26]

$$P(\Phi_B) = \frac{1}{\sigma_s \sqrt{2\pi}} \exp\left(-\frac{(\Phi - \Phi_B)^2}{2\sigma_s^2}\right) \quad (5)$$

where $I_s(\Phi)$ is the normalization constant of the Gaussian barrier height distribution, the total current across a Schottky diode containing barrier inhomogeneities can be expressed as [27]:

$$I(V) = \int I_s(\Phi) P(\Phi) \exp\left(\frac{q(V - \Phi)}{kT}\right) d\Phi \quad (6)$$

where $I_s(\Phi)$ is the current at a bias V for a barrier of height based on the ideal thermionic emission diffusion (TED) theory and $P(\Phi)$ is the normalized distribution function giving the probability of accuracy for barrier height. Performing this integration, one can obtain the current $I(V)$ through a Schottky barrier at a forward bias but with a modified barrier as

$$I(V) = I_0 \exp\left(\frac{qV}{kT}\right) \left[1 - \exp\left(-\frac{qV}{kT}\right)\right]^{n_{ap}} \quad (7)$$

with

$$I_0 = A A^{**} T^2 \exp\left(-\frac{q\Phi_{B0}}{kT}\right) \quad (8)$$

where Φ_{ap} and n_{ap} are the apparent barrier height at zero bias and apparent ideality factor, respectively given by [25], [28]

$$\Phi_{ap} = \Phi_{B0} + \frac{2\sigma_s^2}{q} \quad (9)$$

$$\left(\frac{1}{n} - 1 \right) \frac{q}{2kT} = \frac{B_0}{2kT} + \frac{s_0}{2kT} \quad (10)$$

We need to assume that the mean Schottky barrier height B_0 and s_0 are linearly bias-dependent on Gaussian parameters, such that $B_0 = B_0(T=0) + \alpha_2 V$ and standard deviation $s_0 = s_0(T=0) + \alpha_3 V$, where α_2 and α_3 are voltage coefficients which may depend on temperature [29]. The temperature dependence of s_0 is small and therefore can be neglected [30].

We attempted to draw a B_0 versus $q/2kT$ plot (Fig. 5) to obtain the value of the GD of the barrier heights and from the intercept and the slope the values of B_0 and s_0 are 1.753eV and 0.225 respectively. The structure with the best rectifying performance presents the best barrier homogeneity with the lower value of the standard deviation. It was seen that the value of s_0 is not small compared to the mean value values of B_0 , and it indicates the presence of interface inhomogeneities. Therefore, the plot of $[1/(n)-1]$ versus $q/2kT$ should be a straight line that gives the voltage coefficients $\alpha_2=0.161V$ and $\alpha_3=0.038V$ from the intercept and slope, respectively (as shown in Fig. 5). Now, by combining (8) and (9), the Richardson plot can be modified to

$$\ln \left(\frac{I_0}{T^2} \right) - \frac{q^2 s_0^2}{2k^2 T^2} = \ln(AA^{**}) - \frac{qB_0}{kT} \quad (11)$$

The plot of the modified $\ln(I_0/T^2) - q^2 s_0^2 / 2k^2 T^2$ versus q/kT , should give a straight line with the slope directly yielding the mean B_0 as 1.78 eV and the intercept ($\ln AA^{**}$) at the ordinate determining A^{**} for a given diode area A as 23 A/cm² K² (as seen in Fig. 6), respectively, without using the temperature coefficient of the SBHs. As can be seen, $B_0=1.78$ eV from this plot according to (11), in good agreement with the value of $B_0=1.75$ eV from B_0 versus q/kT (Fig. 5). Therefore, it can be concluded that the temperature dependence of the forward $I-V$ characteristics of the Pd/GaN can be successfully explained based on the thermionic emission mechanism with a Gaussian distribution of barrier heights.

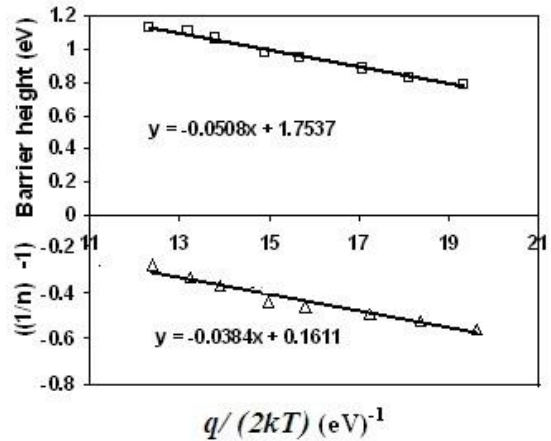


Fig. 5 Zero-bias apparent barrier height and ideality factor versus $q/(2kT)$ curves of the Pd/GaN Schottky diode according to the Gaussian distribution of the barrier heights

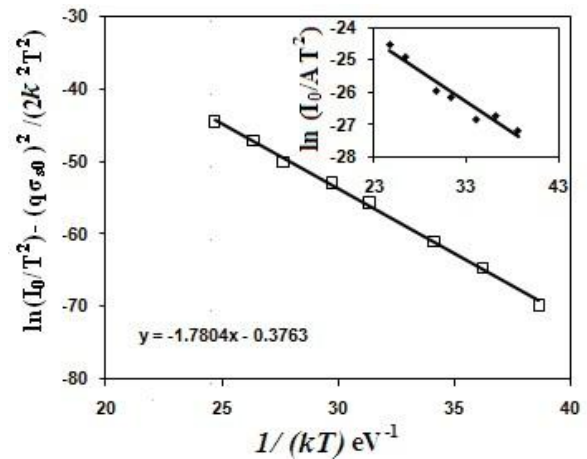


Fig. 6 Modified Richardson plot for the Pd/GaN Schottky diode according to the Gaussian distribution of barrier heights, and before modification shown in the inset

IV. CONCLUSIONS

The $I-V$ characteristics of the Pd/n-GaN contacts were measured in the temperature range 300-470K. Schottky barrier height, ideality factor, saturation current and series resistance of the device characteristics have been found to be strongly dependent on the operating temperature, which could be partly attributed to the inhomogeneities at the metal-semiconductor interface. Barrier height was increased with temperature while ideality factor was decreased which indicated that the diode are dominated by thermionic emission at high temperatures than at low temperatures. The experimental results have showed the non-ideal behavior of the current-transport over the barrier expressed by ideality factors, significantly larger than unity at room temperature and an increasingly effective SBH with rising temperature. The experimental value of Richardson constant ($2.1 \times 10^{-9} \text{ A cm}^{-2} \text{ K}^{-2}$) is much lower than the known theoretical value of $26 \text{ A cm}^{-2} \text{ K}^{-2}$ for n-GaN, but after the thermionic emission theory was modified by

Gaussian distribution (GD) we obtained the value of 23 Acm^{-2} -2

K which is very closed to theoretical value. Therefore, it can be concluded that the temperature dependence of the forward I - V characteristics of the Pd/GaN can be successfully explained based on the thermionic emission mechanism with a Gaussian distribution of barrier heights.

REFERENCES

- [1] H. Morkoc, S. Strite, G.B. Gao, M.E. Lin, B. Sverdlov, M. Burns, *J. Appl. Phys.*, vol. 76, pp. 1363, 1994.
- [2] J. D. Guo, M. S. Feng, R. J. Guo, F. M. Pan, C. Y. Chang, *Appl. Phys. Lett.* Vol. 67, pp 2657, 1995.
- [3] L. Wang, M. Y. Nathan, T. H. Lim, M. A. Khan, Q. Chen, *Appl. Phys. Lett.* Vol. 68, pp 1267, 1996.
- [4] K. Suzue, S. N. Mohammad, Z. F. Fan, W. Kim, O. Aktas, A. E. Botchkarev, H. Morkoc, *J. Appl. Phys.* Vol. 80, pp. 4467, 1996.
- [5] Q. Z. Liu, L. S. Yu, S. S. Lau, J. M. Redwing, N. R. Perkins, T. F. Kuoch, *Appl. Phys. Lett.* vol 70, pp. 1275, 1997.
- [6] S. C. Binari, K. Doverspike, G. Kelner, H. B. Dietrich, A. E. Wickenden, *Solid-State Electron.* Vol. 41, pp. 177, 1997.
- [7] C.K. Tan, A. Abdul Aziz, F.K. Yam, *Applied Surface Science.* Vol. 252, pp. 5930, 2006.
- [8] B. Deba, A. Ganguly, S. Chaudhuri, B.R. Chakraborti, A.K. Pal.
- [9] B. Akkal, Z. Benamara, H. Abid, A. Talbi, B. Gruzza, *Materials Chemistry and Physics.* Vol. 85, pp. 27 2004.
- [10] J. Osvald, J. Kuzmik, G. Konstantinidis, P. Lobotka, A. Georgakilas, *Microelectronic Engineering.* Vol. 81, pp. 181, 2005.
- [11] A. R. Arehart, B. Moran, J. S. Speck, U. K. Mishra, S. P. Den Baars, S. A. Ringel, *J. Appl. Phys.* Vol. 100, pp. 023709, 2006.
- [12] Z. Tekeli, . Altndal, M. Çakmak, S. Özçelik, *J. Appl. Phys.* Vol. 102, pp. 054510, 2007.
- [13] M. Ravinandan, P. Koteswara Rao, V. Rajagopal Reddy, *Semicond. Sci. Technol.* Vol.24, pp. 035004, 2009.
- [14] E. H. Rhoderick, R. H. Williams, *Metal Semiconductor Contacts* second ed., (Oxford: Oxford University Press) (1988).
- [15] P. Koteswara Rao, V. Rajagopal Reddy. *Materials Chemistry and Physics.* Vol. 114, pp. 821, 2009.
- [16] Yu-Zung Chiou , Jung-Ran Chiou , Yan-Kuin Su, Shouu-Jinn Chang,Bohr-Ran Huang, Chia-Sheng Chang, Yi-Chao Lin *Materials Chemistry and Physics.* Vol. 80, pp. 201, 2003.
- [17] Y. Kribes, I. Harrison, B. Tuck, T.S. Cheng, C.T. Foxon, *Semicond. Sci. Technol.* vol. 12, pp. 913, 997.
- [18] J.D. Guo, F.M. Pan, M.S. Feng, R.J. Guo, R.F. Chou, C.Y. Chang, *J. Appl. Phys.* Vol.80, pp. 1623, 1996.
- [19] F. Lucolano, F. Roccaforte, F. Giannazzo, V. Raineri, *J. Appl. Phys.* Vo.102, pp. 113, 2007.
- [20] F. Roccaforte, F. La Via, V. Raineri, R. Pierobon, E. Zanoni, *J. Appl. Phys.* Vol. 93, pp. 9137, 2003.
- [21] J S. Altindal, S. Karadeniz, N. Tougluoglu, A. Tataroglu, *Solid-State Electron.* Vol. 47, pp. 1847, 2003.
- [22] Y.P.Song, R.L.Meirhaeghe, W.H.Laflere, F.Cardon, *Solid State*
- [23] S. Zeyrek, S. Altndal, H. Yüzer, M. M. Bülbül, *Appl. Surf. Sci.* vol. 252, pp. 2999, 2006.
- [24] S. Zhu, R. L. VanMeirhaege, C. Detavernier, F. Cardon, G. P. Ru, X. P. Qu, B. Z. Li, *Solid State Electron.* Vol. 44, pp. 663, 2000.
- [25] M. K. Hudait, S. P. Venkateswarlu, S. B. Krupanidhi, *Solid State Electron.* Vol. 45, pp. 133, 2001.