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# Study of the surface state density and potential in MIS diode Schottky using the surface photovoltage method

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## ABSTRACT

The effects of surface preparation and illumination on electric parameters of Au/GaN/GaAs Schottky diode were investigated. The thin GaN film is realized by nitridation of GaAs substrates with different thicknesses of GaN layers (0.7 – 2.2 nm). In order to study the electrical characteristics under illumination, we use an He-Ne laser of 632 nm wavelength. The I(V) current- voltage, the surface photovoltage SPV measurement were plotted and analysed taking into consideration the influence of charge exchange between a continuum of the surface states and the semiconductor. The barrier height  $\Phi_{bn}$ , the serial resistance  $R_s$  and the ideality factor  $n$  are respectively equal to 0.66 eV, 1980  $\Omega$ , 2.75 under dark and to 0.65 eV, 1160  $\Omega$ , 2.74 under illumination for sample 1 (GaN thickness of 0.7 nm). The interface states density  $N_{ss}$  in the gap and the excess of concentration  $\delta n$  are determined by fitting the experimental curves of the surface photovoltage SPV with the theoretical ones and are equal to  $4.5 \times 10^{12} \text{ eV}^{-1} \text{ cm}^{-2}$ ,  $5 \times 10^7 \text{ cm}^{-3}$ , respectively, for sample 1 and  $3.5 \times 10^{12} \text{ eV}^{-1} \text{ cm}^{-2}$ ,  $7 \times 10^8 \text{ cm}^{-3}$  for sample 2 (GaN thickness of 2 nm). The results confirm that the surface photovoltage is an efficient method for optical and electrical characterizations.



## KEYWORDS

SPV; laser; Nitridation; Characterization

## 1. Introduction

The surface state density (SSD) and the barrier height (BH) of the MIS Schottky diode are important parameters, which influence the performance of devices. We have several methods for measuring the SSD such as the current – voltage, capacitance - voltage [1] and surface photovoltage SPV method. The surface photovoltage was first introduced by A. M. Goodman in 1961 [2] for measuring minority carrier diffusion lengths in extrinsic semiconductors. In surface photovoltage one measures the change in the surface potential due to optically excited electron hole pair generation under periodic illumination and subsequent carrier redistribution and/or recombination in the surface states [3]. The surface photovoltage has emerged as a powerful method to study surface states, heterojunction, quantum well, and other nanostructures.

The propose of this paper is to characterize the interface states in Au/GaN/GaAs Schottky diode using the surface photovoltage method.

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**Table 1.** Conditions of elaboration and estimations of created GaN thickness.

	Nitridation time	GaN thickness
Sample 1	5 min	0.7 nm
Sample 2	30 min	2.2 nm

## 2. Experimental part

The commercially available GaAs (001) wafers are n-type with concentration  $N_D = 4.9 \times 10^{15} \text{ cm}^{-3}$ . The cleaning procedure of the samples consists of 3 steps:

Step 1: chemical cleaning subsequently in  $\text{H}_2\text{SO}_4$ , deionized water, cold and hot methanol all combined with ultrasounds, finally drying in  $\text{N}_2$ ,

Step 2:  $\text{Ar}^+$  ion bombardment (ion energy: 1 keV, sample current:  $5 \mu\text{A}/\text{cm}^2$ , time: 1 h) in UHV chamber,

Step 3: sample heating at  $500^\circ\text{C}$  in UHV chamber.

A singular glow discharge source (GDS) described in detail elsewhere [4] was used for the nitridation. In this kind of nitrogen cell which presents the particularity of working at low power (5–10 W) continuous plasma was produced by a high voltage (about 2.5 kV) and a majority of N atomic species were created (nitrogen pressure:  $1 \times 10^{-2}$  Pa, sample current:  $1.0 \mu\text{Acm}^{-2}$ ). Nitridation was made at a power range of 5 W during 5 and 30 min in the same UHV chamber of steps 2 and 3. The sample temperature was kept at  $500^\circ\text{C}$  during the nitridation.

All the samples were analyzed *in situ* by XPS. These experiments were carried out in an UHV chamber equipped with an XPS system (dual anode Al–Mg X-ray source and hemispherical electron energy analyzer OMICRON EA125). Mg  $K\alpha$  source (1253.6 eV) at an incident angle of  $55^\circ$ , normal detection and pass energy of the analyzer equal to 20 eV were used for analysis. Estimation of the created GaN thickness was made using models described elsewhere [5].

Nitridation time and estimations of created GaN thicknesses on GaAs are summarized in Table 1.

After the nitridation steps, *in situ* deposition of a  $750 \mu\text{m}$ -diameter and 100 nm-thick Au dot was realized. Then, after removing the sample from the UHV chamber, Tin was deposited on the back face with  $\text{N}_4\text{HCl}$  in order to improve the quality of the Ohmic contacts. The sample was heated to a temperature of  $350^\circ\text{C}$  during 5 minutes to allow the diffusion of Tin in GaAs.

Then these structures were electrically tested. The measurements of current versus bias voltage  $I(V)$  in the dark and under illumination (monochromatic light  $\lambda = 632 \text{ nm}$ ) were obtained using an HP Semiconductor Parameters Analyzer 4155B.

## 3. Theoretical part

If the semiconductor is no generated, we obtain the relation of the electron and hole densities in space charge region (SCR) to their densities in the quasi neutral bulk from the Boltzmann relation [3]:

$$n(x) = n_b e^{\psi_0(x)} \quad (1)$$

$$p(x) = p_b e^{\psi_0(x)} \quad (2)$$

where  $\psi_0(x)$  is the electrostatic potential in units of  $kT/q$  in the dark condition.

$k$ ,  $T$ ,  $q$  are the Boltzmann constant, the temperature in Kelvin and the electron charge respectively.

$n_b$ ,  $p_b$  are the thermodynamic equilibrium densities of holes and electrons in bulk respectively.

In the presence of both donors and acceptors, the total charge density is [3]:

$$\rho(x) = q[N_d - N_a + p(x) - n(x)] \quad (3)$$

where  $N_d$ ,  $N_a$  are the donor and acceptor density respectively.

In the quasi neutral region, the net charge density is zero.

$$N_d - N_a = n_b - p_b \quad (4)$$

The space charge is obtained by solving Poisson's equation; the explicit expression for the charge  $Q_{sc}$  is [6]:

$$Q_{sc} = A \frac{|\psi_0|}{\psi_0} [\beta (e^{-\psi_0} - 1) + \beta^{-1} (e^{\psi_0} - 1) + (\beta + \beta^{-1}) \psi_0]^{1/2} \quad (5)$$

where:  $A = -(2n_i \epsilon_s kT)^{1/2}$   $\beta$  is the doping factor (ratio of  $p_0/n_i$ ),  $n_i$  the intrinsic concentration,  $p_0$  bulk hole concentration in equilibrium and  $\epsilon_s$  is the semiconductor permittivity.

The surface photovoltage  $\Delta\psi$  is defined as difference of surface potential in nonequilibrium (under illumination) and equilibrium (under dark) [6].

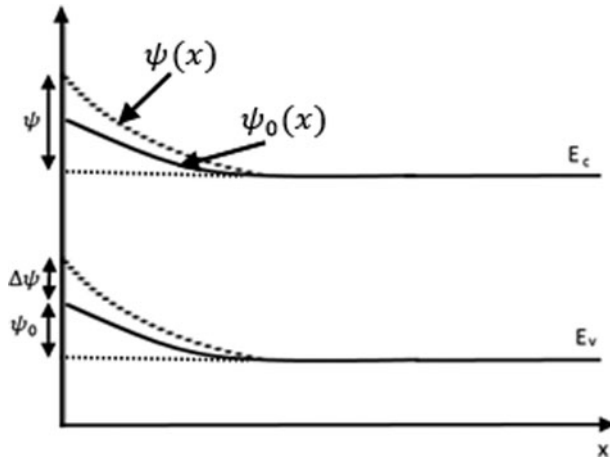
$$SPV = \Delta\psi = \psi - \psi_0 \quad (6)$$

where  $\psi$  is the surface potential under illumination and  $\psi_0$  is the surface potential under dark (see Fig. 1).

The electrostatic potential under dark  $\psi_0(x)$  is given by: [7]

$$\psi_0(x) = (V - V_d) \times \left( \frac{2x}{W} - \frac{x^2}{W^2} \right) \quad (7)$$

Where  $V$  is the applied voltage,  $V_d$  the diffusion potential,  $x$  the distance from surface and  $W$  the depletion zone width.



**Figure 1.** Energetic band diagram.

Under illumination, the absorbed photos induce the formation of free carriers by creating electron-hole pairs via band to band transitions and/or release captured carriers via trap- to band transitions. The photo generated excess carrier concentrations for electrons and holes are given by [6]:

$$\delta n(x) = n(x) - n_0 \quad (8)$$

$$\delta p(x) = p(x) - p_0 \quad (9)$$

The charges,  $Q_{sc}$  and  $Q_{ss}$  under illumination change due to both carrier injection and charge in surface potential. Therefore, the differential of the charge neutrality condition may be written as [3]:

$$\delta Q_{sc} = \delta Q_{ss} \quad (10)$$

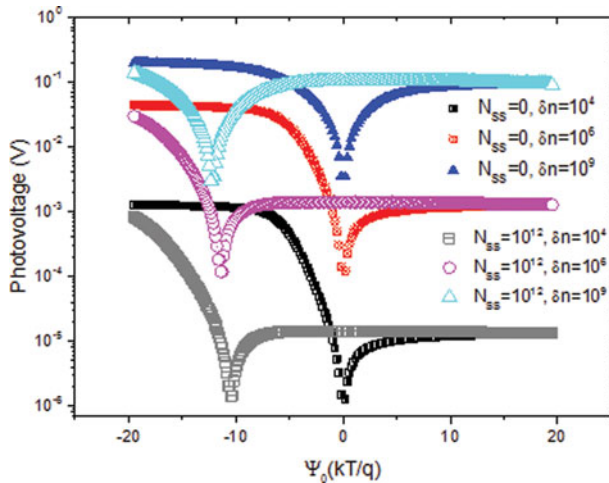
where  $\delta Q_{sc}$  is the change of charge inside the space charge region under illumination and  $\delta Q_{ss}$  the corresponding change of charge in surface states.

Therefore, we expressed Eq. (10) as a function of surface photovoltage  $\Delta\psi$  and interface state density  $N_{ss}$  by [6]:

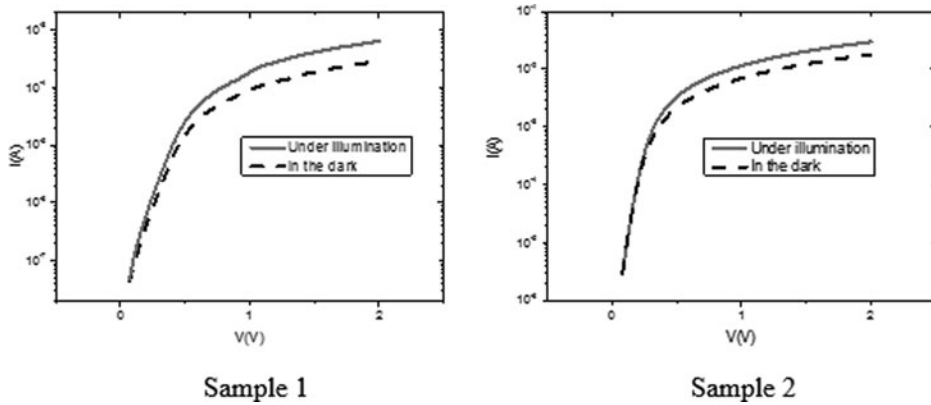
$$\begin{aligned} & A \frac{|\psi|}{\psi} \left[ \beta (e^{-\psi} - 1) + \beta^{-1} (e^{\psi} - 1) + (\beta + \beta^{-1}) \psi + \frac{\delta n}{n_i} (e^{\psi} + e^{-\psi} - 2) \right]^{1/2} \\ & - A \frac{|\psi_0|}{\psi_0} \left[ \beta (e^{-\psi_0} - 1) + \beta^{-1} (e^{\psi_0} - 1) + (\beta + \beta^{-1}) \psi_0 \right]^{1/2} + qkTN_{ss} \\ & \left[ -\ln \left( 1 + \frac{\delta n}{n_i \beta} - \Delta\psi \right) \right] = 0 \end{aligned} \quad (11)$$

Using parameters pertaining to GaAs at room temperature ( $n_i = 1.79 \times 10^6 \text{ cm}^{-3}$ ,  $\epsilon_s = 12.9 \text{ Fcm}^{-1}$ ), solutions of Eq. (11) have been plotted in Fig 2.

Curves (see Fig 2) show that the parameters  $N_{ss}$  and  $\delta n$  have marked influence on the photovoltage. For the interface states density, the curves have been horizontally shifted and for excess concentration, they were vertically shifted.



**Figure 2.** Calculated photovoltages as function of band bending for two values of the surface states density  $N_{ss}$  and three values of excess concentration  $\delta n$ .



**Figure 3.**  $I(V)$  Characteristics in the dark and under illumination.

#### 4. Results and discussion

The direct measured  $I(V)$  under dark and illumination is shown in [fig. 3](#) for simple 1 and simple 2. The difference between the under dark case and the illumination one is important for bias  $V > 1$  V. This seems to be due to the generation-recombination phenomenon. It occurs, consequently from free charges creation in excess ( $\delta p = \delta n$ ), hence, an increase in the  $N_d$  impurity concentration. This effect is a direct influence on the parameters bound to  $N_d$ , such as the saturation current  $I_s$ , the barrier height  $\phi_{Bn}$  and the serial resistance  $R_s$ .

The determination of the electric parameters was achieved using the characteristic formula expressing the thermoionic emission current passing through a Schottky diode [1, 8]:

$$I_{th} = I_s e^{\frac{q(V - R_s I_{th})}{nkT}} \text{ for } V > \frac{3kT}{q} \quad (12)$$

where  $n$  is the ideality factor and  $I_s$ , the saturation current density. The saturation current density can be expressed by:

$$I_s = A * T^2 e^{\frac{-q\phi_{Bno}}{kT}} \quad (13)$$

Where  $\Phi_{Bno}$ ,  $A*$ , are the barrier height at zero bias and the effective Recharadson constant which is equal to  $8,78 \text{ A cm}^{-2} \text{ K}^{-2}$  [1] respectively.

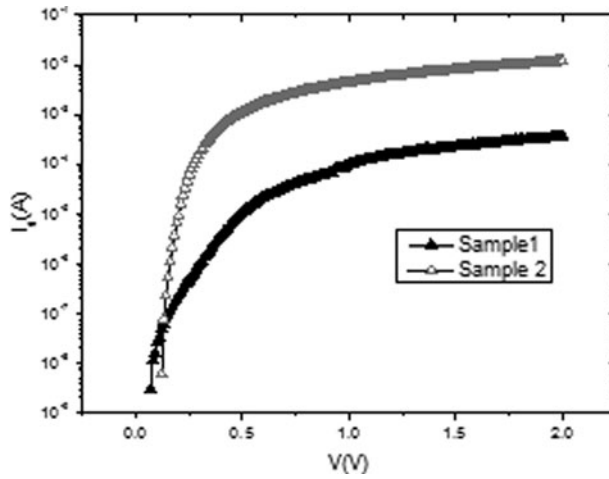
From the  $\ln(I) = f(V)$  curves, we estimated the saturation current  $I_s$ , the ideality factor  $n$ , the barrier height  $\Phi_{Bn}$  and the serial resistance  $R_s$  for both of sample in the dark and under illumination.

The electrical parameters obtained for both of simples are reported in [table 2](#).

The increase of the saturation current under illumination du to the transfert of the photo generated electrons and holes. But the decrease of resistance under illumination is associated with the generation of charge carriers.

**Table 2.** Experimental parameters extracted under dark and under illumination using  $I(V)$  measurements.

	Under Dark				Under illumination			
	$I_s$ (A)	$n$	$\Phi_{Bn}$ (V)	$R_s$ ( $\Omega$ )	$I_s$ (A)	$n$	$\Phi_{Bn}$ (V)	$R_s$ ( $\Omega$ )
Sample 1	$2.33 \times 10^{-8}$	2.75	0.66	$1.98 \times 10^3$	$3.74 \times 10^{-8}$	2.74	0.65	$1.16 \times 10^3$
Sample 2	$3.45 \times 10^{-7}$	1.34	0.60	74.56	$3.59 \times 10^{-7}$	1.33	0.59	48.24



**Figure 4.** Generation current variations as a function of bias voltage.

The generation current is the difference between the current under illumination and the current in the dark, it can be written as:

$$I_g = I_{ph} - I_{dark} \quad (14)$$

Where  $I_{dark}$  and  $I_{ph}$  are the current in the dark and under illumination respectively.  $I_g$  curves are plotted in Fig 4.

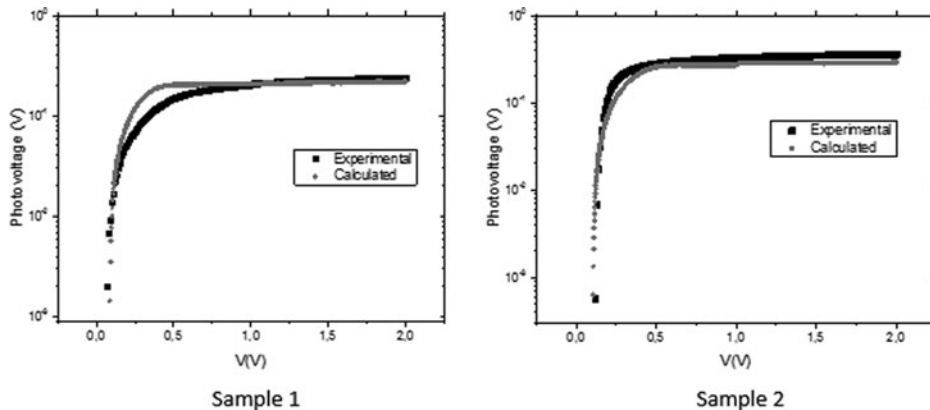
Curves in fig 4. show that the generation current for sample 2 is more important than that shown for sample 1.

The experimental SPV can be evaluated by: [9]

$$SPV = \frac{nkT}{q} \ln \left( 1 + \frac{I_g}{I_s} \right) \quad (15)$$

Values of the interface state density  $N_{ss}$  and the excess concentration  $\delta n$ , for both of samples, can be determined after fitting the SPV experimental curves with those calculated theoretically.

Values of the interface states density and the excess concentration, obtained from SPV method were recapitulated in Table 3.



**Figure 5.** SPV experimental curves plotted and fitted with calculated ones.

**Table 3.** Values of interface state density and excess concentration obtained by SPV method.

	SPV method	
	$N_{ss} \text{ (cm}^{-2}\text{eV}^{-1}\text{)}$	$\delta n \text{ (cm}^{-3}\text{)}$
Sample 1	$4.5 \times 10^{12}$	$5 \times 10^7$
Sample 2	$3.5 \times 10^{12}$	$7 \times 10^8$

Results show that sample 1 presents a higher interface states density than sample 2 this may be explained by the presence of a large number of traps and defects due to the insufficient of the thickness of the GaN layer.

Sample 2 presents better electrical parameters compared to sample 1. This can be attributed to the improvement of the GaAs surface quality after 30 min of nitridation.

The used laser energy of 1.96 eV which is greater the band gap energy of the GaAs, is sufficient to extract the valence band electrons. The excess of concentration  $\delta n$  can be calculated from [10]:

$$\delta n = \delta p = \frac{J_{ph} R_s C_{sc}}{q} \quad (16)$$

where  $J_{ph}$  is photo current and  $C_{sc}$  the capacitance of the semiconductor.

Values of excess concentration  $\delta n$  from Eq.(16) for sample 1 and 2 are  $3.57 \times 10^7 \text{ cm}^{-3}$  and  $2.48 \times 10^8 \text{ cm}^{-3}$  respectively. These results are in good agreement with those obtained using SPV method.

## Conclusion

The article presents an electrical study of the surface states density and the potential in elaborated components after Au/GaN/GaAs using the surface photovoltage method.

Electrical parameters of ideality factor  $n$ , current of saturation  $I_s$ , serial resistance  $R_s$ , the barrier height  $\Phi_{Bn}$  and the diffusion potential  $V_d$  were calculated using  $I(V)$  in the dark and under illumination and  $C(V)$  measurements.

The resistance which decreases under illumination is close to the electrons, we know that the resistance is inversely proportional to the doping level.

The state density in the band gap is widely reduced with increasing of the nitridation time from 5 min (sample 1) to 30 min (sample 2) of nitridation.

The improvement of the electrical parameters after 30 min of nitridation shows that the GaN with a thickness of 2 nm presents a good passivation for the GaAs surface.

SPV experimental results are in good agreement with those obtained from the theoretical model. Therefore, the surface photovoltage is an efficient method of electrical and optical characterizations.



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