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Jaime Mimila-Arroyo, Alma Sofía Arreola-Pina, François Jomard, Alain Lusson. Effect of the plasma experimental parameters on the dose and profiles of hydrogen in-diffused into the GaN/AlGaN/GaN/Si high electron mobility transistor. *Materials Science and Engineering: B*, 2023, 290, 10.1016/j.mseb.2023.116279 . hal-04233280

**HAL Id: hal-04233280**

**<https://hal.science/hal-04233280>**

Submitted on 3 Nov 2023

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# EFFECT OF THE PLASMA EXPERIMENTAL PARAMETERS ON THE DOSE AND PROFILES OF HYDROGEN IN-DIFFUSED INTO THE GaN/AlGa<sub>N</sub>/Ga<sub>N</sub>/Si HIGH ELECTRON MOBILITY TRANSISTOR

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## **Abstract**

The structures of electronic devices based on GaN and its AlGa<sub>N</sub> alloys grown on foreign substrates, display a high threading dislocations concentration (TDs);  $10^7$ - $10^{11}$  cm<sup>-2</sup>. They introduce deleterious effects diminishing the devices predicted performances. The High Electron Mobility Transistor (HEMT) core is constituted by an AlGa<sub>N</sub>/Ga<sub>N</sub> heterojunction, where the AlGa<sub>N</sub> layer, of nanometric dimensions, results on the formation of the high mobility two-dimensional electron gas (TEG), conducting channel of the device. The performance of this transistor has been improved by its proper hydrogenation, although the process can, as well, catastrophically degrade the device. As the hydrogenation has not been studied in detail neither optimized to improve the device performance, here is presented a detailed study of the effect of the hydrogenation experimental parameters: plasma power, sample temperature and duration, on its dose and distribution throughout the structure. The study is focused on the conditions that might lead to a hydrogen distribution and dose that improve the HEMT charge transport properties and practiced on HEMT structures coming from three different vendors, grown on Si substrates by molecular beam and MOCVD epitaxy. Hydrogen profiles and dose were obtained by Secondary Ion Mass Spectroscopy. The hydrogen profiles allow a clear identification of the different layers and structure interfaces. The dose depends on the square of the plasma power, increases linearly on the hydrogenation time and slightly proportional to the sample temperature.

Interestingly a hydrogen peak concentration is systematically obtained at the AlGa<sub>N</sub>/Ga<sub>N</sub> interface beneath where the two-dimensional electron gas lays, revealing a highly defective interface degrading the electron gas physic performances and whose defect concentration seems to be dependent on the epitaxial technique. These results shed light on how to improve the AlGa<sub>N</sub>/Ga<sub>N</sub> HEMT performance and allow to tailor the experimental plasma conditions to do so through a simple and short hydrogenation process.

Key words: HEMT, Gallium nitride, Hydrogenation-Dose, Plasma

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## 1 INTRODUCTION

The structures of some electronic devices based on GaN and its AlGaN alloys are usually grown on foreign substrates as; sapphire, Silicon carbide, silicon, zinc oxide, and others with which a large lattice and thermal mismatch exist. The obtained material results highly defective displaying a typical threading dislocations concentration (TDs) in the range of  $10^7$ - $10^{11}$   $\text{cm}^{-2}$ . [1 – 3]. TDs in these materials constitute a line of dangling bonds linked to gallium vacancies that behave like acceptors. Additionally, around the TDs core there is a high concentration of acceptor-like defects that capture free electrons as well, constituting together a negative rod with a radius of several nanometers that might bear a charge density as high as  $10^{20}$   $\text{cm}^{-3}$ , forming a built-in energy barrier, which is highly efficient at scattering and recombining carriers [4-8]. Such concentration of extended defects strongly degrades the GaN and AlGaN physical properties, abnormally decreasing its mobility, photoluminescence yield, producing the persistent photoconductivity as well as other deleterious effects [9- 12]. All this results on devices performance lower than expected. Notwithstanding this drawback, high performance devices are being successfully developed with GaN and its AlGaN alloys. For the AlGaN/GaN High Electron Mobility Transistor (HEMT) such defects introduce deleterious effects, as the drain current knee walk out, its collapse, gate lag, reduction of the breakdown voltage and  $1/f$  noise increase, among others [13, 15]. The structure of this HEMT comprises the adapting layers to the foreign substrate followed by a several micrometers thick layer of unintentionally doped GaN (UID), a  $\sim 20$  nm thick layer of UID AlGaN and finally a  $\sim 1.0$  nm of UID GaN. The nanometric AlGaN layer on top of the GaN results on the spontaneous formation of the high mobility two-dimensional electron gas (TEG) constituting the HEMT conduction channel, located beneath the AlGaN layer but completely contained in the GaN and confined against the AlGaN-GaN interface. The electron mobility in the TEG depends, mainly, on the TDs concentration at its location and the AlGaN/GaN interphase rugosity, if any, which might strongly degrade the TEG electrical properties [16]. The TEG is characterized by a high free electron concentration  $\sim 10^{13}$   $\text{e}/\text{cm}^2$  whose mobility is around  $\sim 1500$   $\text{cm}^2/\text{V}\cdot\text{sec}$ , leading to a device displaying

outstanding performance for high frequency and power electronics [17, 18]. Additionally, as AlGaIn and GaN are wide bandgap materials this HEMT can operate at high temperature.

By another way it has been well established that hydrogen, in some semiconductors, might interact with impurities and defects passivating them. In some cases, resulting as if the defects or impurities had been totally “suppressed” [19]. In the case of GaN it is well known that hydrogen might passivate some acceptor impurities and acceptor-like defects, with no reports of donor passivation. It has been reported that through their hydrogenation the physical properties of unintentionally doped n-type GaN epitaxial layers, are strongly improved increasing their photoluminescence yield and electron mobility, reducing the residual free electron concentration, and making almost disappear the persistent photoconductivity. These effects have been associated to the partial passivation of acceptor defects around the TDs. In the passivation mechanism, hydrogen might bond mainly to ionized acceptors located at or around the dislocation edge;  $A_d^-$  and  $A^-$ , respectively, forming complexes and freeing electrons, according to Eq. (1)



where  $A^-$  is an ionized acceptor-like defect or impurity, wherever located. The hydrogen passivation of acceptors located at and around the dislocation core reduces the negative charge in it, decreasing the height of the built-in energy barrier, the size of its space charge region, and its deleterious effects, improving devices performance. Additionally, unbounded hydrogen, which in n-type GaN behaves like an acceptor, captures free electrons decreasing its residual concentration. It has been demonstrated that by its proper hydrogenation the charge transport properties of this HEMT might be improved: typically, 30% increase in the free electron channel concentration with a slight increase on its mobility, associated with the smoothing of the AlGaIn/GaN interphase, etc. [20-27]. Such improvements remain stable at temperatures close to 800 °C. Moreover, the performance of this device is quite heterogenous throughout a two- or three-inches wafer and systematically it has been observed that

its hydrogenation homogenizes its performance at the hydrogen improved level throughout the entire wafer, as well as its reliability, improvements that remain stable at high temperatures [28, 29]. The observed increase of the TEG free electron concentration, after a proper hydrogenation of the structure, when the in-diffused hydrogen locates on the structure surface, and the top GaN and AlGa<sub>N</sub> layers without reaching the TEG region. This implies that in this HEMT structure its surface and its top layers contain an important concentration of ionized acceptors, that when passivated by the hydrogen, release their captured electrons, Eq. (1), which go to the conducting channel. On the contrary, if the hydrogen dose is too high and reaches the TEG region, because of the H acceptor behavior in n-GaN, it captures free electrons, reducing their concentration and their mobility, as H<sup>-</sup> dispersion centers are introduced. Although, the same process to in-diffuse the hydrogen into the HEMT structure can catastrophically degrade its charge transport properties, depending on the hydrogen dose and its distribution throughout the structure [30]. Then, to improve the TEG charge transport properties of this HEMT two restrictions must be satisfied: the hydrogen dose should be close to the total quantity of ionized acceptors contained in the structure top layers; GaN, AlGa<sub>N</sub> and its surface. Additionally, the hydrogen distribution throughout the structure must be such that it should remain in those layers, without reaching the two-dimensional electron gas region [25, 26]. To satisfy these requirements some knowledge of the physics of the hydrogen in-diffusion in this structure is needed. However, despite the promising and encouraging results already reported in the literature little attention has been dedicated to the study of the hydrogenation procedure to improve the performance and reliability of this HEMT.

Here is presented a detailed study of the effect of the experimental parameters: plasma power, sample temperature and hydrogenation duration, on its dose and distribution throughout the HEMT structure. This study is badly needed and focuses on the hydrogenation conditions that might lead to a dose and distribution that could improve the HEMT charge transport properties. The utilized HEMT structures come from three different vendors, grown on Si substrates by molecular beam and MOCVD epitaxial techniques. The studied HEMTs realized with them are state of the art. Our results show that the dose

of in-diffused hydrogen varies on the square of the plasma power and proportional to the hydrogenation duration although only slightly depending on the sample temperature. The obtained results allow an easy identification of the hydrogenation conditions under which the HEMT structure charge transport properties are improved or on the contrary strongly deteriorated. These results clearly open the possibility of obtaining interesting improvements of the GaN/AlGaIn/GaN/Si HEMT through a simple and easy to realize hydrogenation process.

## **2 EXPERIMENTAL: SAMPLE PREPARATION, H INDIFFUSION AND RESULTS**

The HEMT structures used for this study were grown by Molecular Beam Epitaxy (MBE) on (111) oriented silicon single crystal substrates of 3 inches in diameter. The structure featured, besides the adapting layers, a 1.0  $\mu\text{m}$  thick GaN layer, a 20 nm thick AlGaIn layer, with 25% of Al content, topped with a 1 nm thick GaN layer, all of the layers were unintentionally doped. The as grown structures are completely free of cracks even on the edge of the wafer. Single GaN layers, grown in the same condition as those of the HEMT structure utilized in this study display an n-type conductivity with an electron concentration in the low  $10^{16}$   $\text{e}\text{-cm}^{-3}$ . HEMTs structures from three different vendors were utilized, all of them with the same number of epitaxial layers and corresponding thicknesses. The hydrogenation of the samples was done using the, so called, RF remote plasma method, selected because in it the sample is not placed onto the electrode used to produce the plasma, reducing the potential plasma related damage, instead, the samples were placed 5 cm away from the plasma electrode. The hydrogenation experimental conditions being controlled were plasma power density, sample temperature and in-diffusion duration, the deuterium pressure was kept constant. Plasma power was varied in the range of 1 to 30 Watts, applied through electrodes of 25  $\text{cm}^2$  of area, for a power density in the range of 0.05 to 1.5  $\text{Watts/cm}^2$ . The sample temperature was varied in the range 250  $^{\circ}\text{C}$  to 460  $^{\circ}\text{C}$ , the hydrogenation time from 2.5 to 20 minutes, at a constant hydrogen pressure in the plasma chamber of 1.0 mbar. Once the hydrogenation time was reached the sample holder inside the RF setup was water cooled to room temperature in less than 1.0 minute. Hydrogen profiles and

dose were obtained by SIMS (Secondary Ion Mass Spectroscopy) utilizing a Cameca ims-4f instrument with  $\text{Cs}^+$  primary beam. To have a SIMS detection limit several decades better than for hydrogen, Deuterium (D) was instead in-diffused (SIMS Deuterium detection limit  $\sim 5 \times 10^{15}$  Deuterium- $\text{cm}^{-3}$ ). To obtain absolute concentrations D-implanted standards were employed.

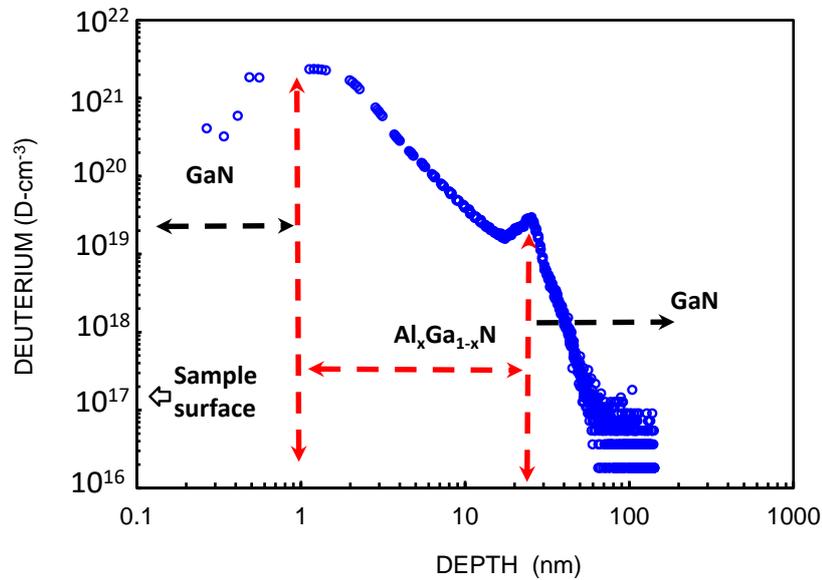


Fig. 1. SIMS Deuterium profile of a HEMT GaN/AlGaN/GaN/Si structure deuterated by the remote plasma method, power plasma 3.0 Watts, sample temperature 260 °C and 10 min. of deuteration.

Figure 1 shows a typical SIMS deuterium concentration profile for a plasma power of 3W, at 260 C and 10 minutes of in-diffusion. As seen, it displays a deuterium concentration behavior clearly different for each semiconducting layer of the HEMT structure, allowing an easy identification of each layer and interfaces between them. From the structure surface to the GaN buffer layer (left to right in the figure) the following layers are identified: The top GaN one, first nanometer, the AlGaN layer, next 20 nm, the AlGaN/GaN interface against which the TEG is confined, the abrupt decrease of the deuterium concentration in the thin GaN region where the TEG is located and the rest of the GaN layer towards the substrate. In the GaN top layer the D concentration starts with a value in the middle  $10^{20}$   $\text{cm}^{-3}$ , increasing towards the first GaN/AlGaN interface, where it reaches its absolute maximum  $\sim 10^{21}$   $\text{cm}^{-3}$ . Then, through the AlGaN layer the deuterium concentration decreases from  $\sim 10^{21}$   $\text{cm}^{-3}$  to  $10^{19}$   $\text{cm}^{-3}$ , in less than 20 nm. In this same AlGaN layer, clearly a few nanometers before the AlGaN/GaN interface

the deuterium reaches its lowest concentration in this layer  $\sim 10^{19} \text{ cm}^{-3}$ , from that point on, the deuterium concentration sharply increases again in a way completely contrary to the diffusion laws. As from that minimum towards the mentioned interface, the D concentration varies going from a low value to a higher one, reaching a secondary maximum, in the low  $10^{19} \text{ cm}^{-3}$ , that seems to occur exactly at the AlGaN/GaN interface. From this metallurgical interface towards the substrate, a sharp decrease in the D concentration is observed going from  $10^{19}$  to  $10^{16} \text{ D/cm}^{-3}$  in just  $\sim 50 \text{ nm}$ . In the remaining of the GaN layer emerges a deuterium plateau with a concentration around  $10^{16} \text{ D-cm}^{-3}$ .

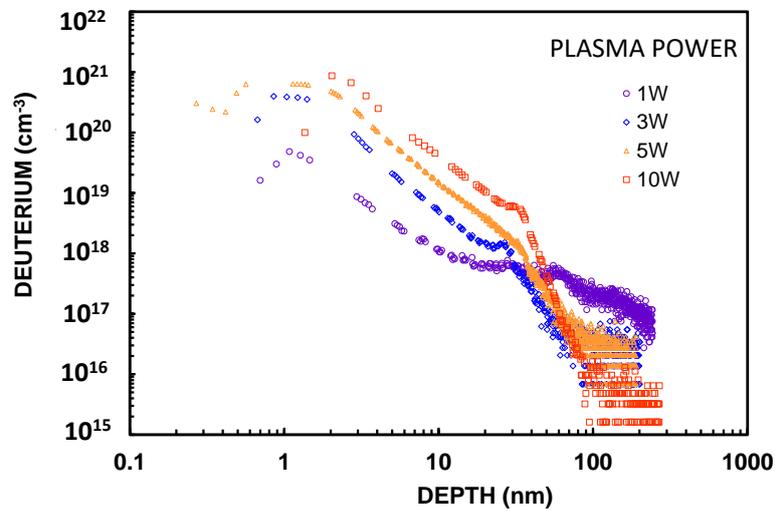


Fig. 2 Deuterium profiles for samples deuterated at different plasma power, at substrate temperature of  $260^\circ\text{C}$  for 10 minutes, other parameters kept constant and the same for each sample.

For all the structures studied, coming from three different vendors, and for all the plasma power utilized, the profiles were quite similar and the AlGaN/GaN interface was always neatly revealed, through a deuterium concentration maximum. Figure 2 shows SIMS deuterium profiles for the HEMT structures, coming from the same wafer, deuterated at four different plasma powers from 1 to 10 Watts, at a substrate temperature of  $260^\circ\text{C}$  and deuteration time constant of 10 minutes. The main features of these profiles are the same as those displayed and described for Fig. 1. However, on Fig. 2 is seen that in the GaN and AlGaN top layers the deuterium concentration profiles shift upwards almost

on a parallel way, as the plasma power increases. An augmentation of the power plasma of one order of magnitude shifts the profile between the top surface and the AlGaIn/GaN interface upwards almost two orders of magnitude. Then, the AlGaIn/GaN interface is always neatly revealed, through a deuterium relative concentration maximum. However, the D profile in the GaN buffer layer from that interface inwards does not shift upwards in a parallel way as the plasma power increases. Instead, it is the deuterium gradient concentration that increases to reach a concentration plateau, around  $10^{16}$  D- $\text{cm}^{-3}$  at a depth around 50 nm, for all the profiles whichever the D concentration at the AlGaIn/GaN interface. Beyond this point, the already mentioned deuterium plateau is systematically obtained, whichever the power plasma, the sample temperature and the deuteration duration, even for a few minutes of hydrogenation duration.

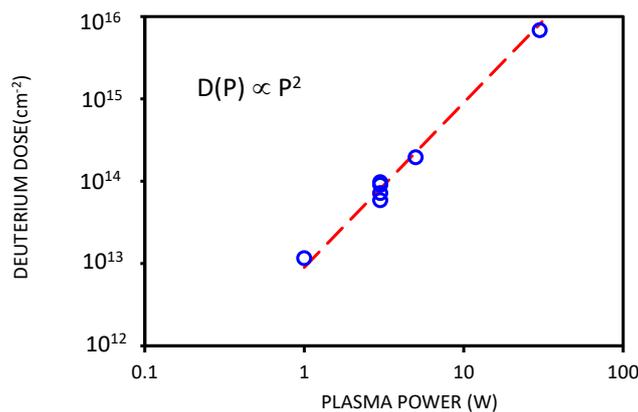


Fig. 3 Deuterium dose as a function of the plasma power. Substrate temperature 260°C and diffusion time 10 min.

The evolution of the deuterium dose as a function of the experimental parameters: power plasma, temperature and deuteration time is shown in Figs. 3, 4 and 5 respectively. The Fig. 3 shows the deuterium dose as a function of the plasma power over one and a half decades, from 1 to 30 Watts, keeping the sample temperature and deuteration duration constants at 260 °C and 10 minutes respectively.

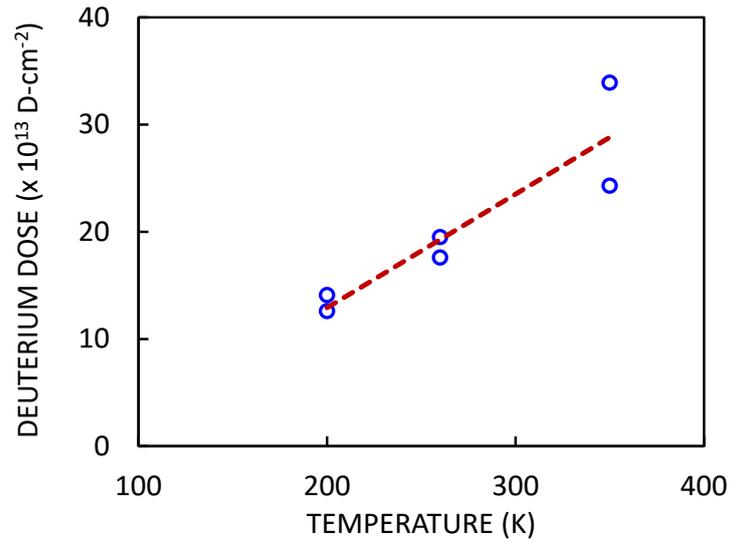


Fig. 4 Deuterium dose as a function of the in-diffusion temperature for a plasma power of 5 Watts and 10 min of hydrogenation time.

The Fig. 4 shows the deuterium dose as a function of the temperature between 200 °C and 350 °C for a power plasma and diffusion time constants at 5 watts and 10 minutes respectively.

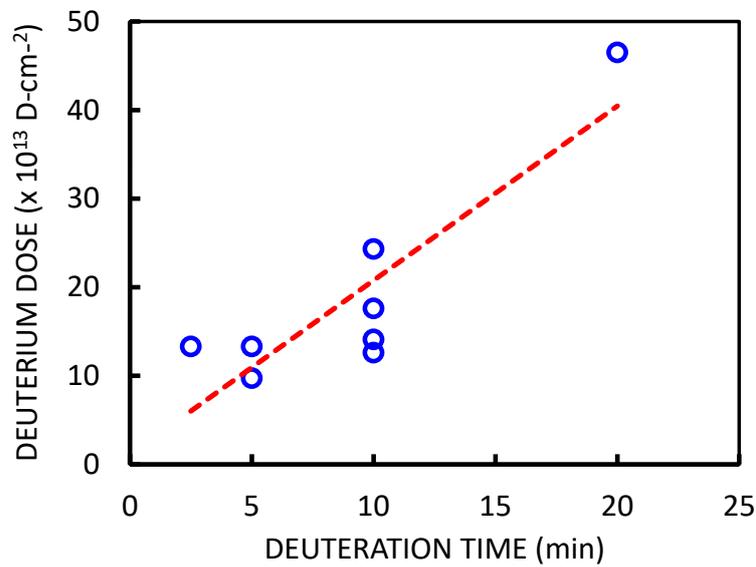


Fig. 5 Deuterium dose as a function of the in-diffusion time a constant plasma power of 5 Watts at 260°C of substrate temperature.

For the Fig. 5, the plasma power and temperature were kept constant at 5 Watts and 260 °C, and the deuteration duration was varied from 2 to 20 minutes.

### 3 DISCUSSION

Hydrogen in GaN is an amphoteric impurity, in p-type GaN behaves like a donor, normally becoming  $H^+$ , in this state of charge it in-diffuses in a normal way. In n-type GaN it becomes  $H^-$ , under such state of charge, it remains almost immobile, as its diffusion activation energy is  $\sim 3.4$  eV, resulting hard to make it to in-diffuse [31]. In this hydrogenation process the  $H^+$  in the plasma surrounds the HEMT structure entering in it and in-diffusing, through two mechanisms. The normal thermally activated and a very fast one which takes place through the highly disordered region around the dislocations [21]. In the deuterated GaN/AlGa<sub>N</sub>/Ga<sub>N</sub>/Si HEMT structure studied here, the deuterium in-diffuses through the top region, where it remains in its initial charge condition as the top layers are almost depleted of free electrons, even if when isolated, are n-type. There, hydrogen might form complexes with ionized acceptors freeing electrons that go to the TEG. Thus, deuterium is found at extremely high concentrations there; around  $10^{20}$  to  $10^{21}$  cm<sup>-3</sup>. In the AlGa<sub>N</sub> layer at one third of its thickness;  $\sim 6.0$  nm, from the AlGa<sub>N</sub>/Ga<sub>N</sub> interface, there is a minimum in the deuterium concentration. From this point towards the interface against which the TEG is confined, the concentration, instead of continuing decreasing according to the diffusion laws, increases. In some samples the deuterium concentration value at the peak, located at the AlGa<sub>N</sub>/Ga<sub>N</sub> interface, can be ten times the value at the minimum. This behavior reveals that this thin region, parallel to the interface AlGa<sub>N</sub>/GAN, contains a high concentration of acceptor-like defects and/or non-intentionally added acceptor impurities, as Gallium vacancies or Carbon at nitrogen site, respectively. It must be remembered that the Gallium vacancy has been found to be a triple acceptor that might bond until four H atoms [34]. The negatively charged acceptor-like defects at the AlGa<sub>N</sub>/Ga<sub>N</sub> interface constitute an extra localized charge that will contribute to the scattering of free electrons as well as to reduce the TEG electrons confinement. The existence of these valley and peak in the deuterium profiles at the AlGa<sub>N</sub> layer was widely confirmed through the realization of many profiles on equal number of different samples with similar structures from three different vendors. Each profile was qualitatively alike although the peak resulted very different in height for different structure origins. For each deuterium atom that bonds to an ionized

acceptor-like defect or impurity, according to Eq. (1), an electron is freed which will increase the TEG free electron concentration, as it has been already reported [25]. By another way the passivation of acceptors at the AlGa<sub>N</sub>/Ga<sub>N</sub> interface and in the thin layer mentioned above decreases the concentration of scattering centers on it as well as the negative fixed charge, resulting on an increase of the channel electron mobility and then, the HEMT ability to handle current and perhaps its frequency response. Additionally, the passivated acceptor states, wherever they could be located will not capture free electrons on a random way anymore, probably decreasing as well, the electrical noise of the structure. The sharp deuterium concentration drop that initiates at the AlGa<sub>N</sub>/Ga<sub>N</sub> interface, actually is not a real one. The SIMS depth resolution is strongly affected by different artifacts due to the sputtering mechanism intrinsic to the technique which normally distorts the profiles, broadening them towards both sides, towards the surface sample and deep into the layer. This effect results because the primary beam relocates atoms, intermixing them [32, 33]. In our study, the obtained D profiles, for the structures from all three vendors, display from the interface towards the substrate, an exponential tail;  $\exp(-x/L_c)$  with a characteristic length  $L_c$  which corresponds to the SIMS depth resolution of our system. At the working conditions utilized in this study; mainly the energy of the primary Cs<sup>+</sup> ions hitting the sample; 14.5 keV, the extracted value is  $L_c = 6.0$  nm [25]. Once the hydrogen reaches the region where electrons are available; the TEG region, it becomes ionized H<sup>-</sup> and almost stops there, not in-diffusing any more, as its diffusion activation energy is high [33]. That explains why the D concentration profile sharply drops at the AlGa<sub>N</sub>/Ga<sub>N</sub> interface, whichever the plasma power. This behavior has been widely experimentally verified, H in n-Ga<sub>N</sub> in-diffuses just in the surface space charge region, where no free electrons are available even at temperatures as high as 460 °C for durations as long as 6 hours [35]. In all the studied samples the long deuterium plateau displaying a deuterium concentration around  $10^{16}$  cm<sup>-3</sup> was observed. Its formation can be due to a strongly localized diffusion mechanism, taking place through the electron depleted space charge region developed around the dislocations core, where the H<sup>+</sup> cannot capture free electrons to become H<sup>-</sup> that

would stop it from diffusing. In that region, due to the high disorder observed around the dislocation core, hydrogen diffuses extremely fast yielding the observed plateau concentration [25].

Figure 3 shows that the in-diffused deuterium dose in these HEMT structures as a function of the plasma power, all other deuteration parameters kept constant, depend on the square of the plasma power. This might indicate that  $H^+$  concentration in the plasma from which the deuterium diffusion is taking place depends, as well, on the square of the RF power producing the plasma. For the dependence of the D dose as a function of the sample temperature during the in-diffusion, Fig. 4 shows a light proportionality with the sample temperature, as when it is increased from 200 °C to 350 °C the deuterium dose increases just two times. Finally, from Fig. 5 the hydrogen dose seems to follow a linear dependence with the deuteration time at least for in-diffusing times smaller than 20 minutes.

#### **4 CONCLUSIONS**

In conclusion, we have presented a detailed study of the dependence of the dose and distribution of hydrogen in the GaN/AlGaN/GaN/Si HEMT structure grown by MBE and MOCVD on Si (111) substrates, as a function of the experimental parameters characterizing the remote plasma in-diffusing technique. The study explores diffusion conditions around those where an improvement on the structure charge transport properties might be obtained. Although our results can be extrapolated for when hydrogenation conditions are such that the hydrogen reaches the TEG and degrades it reducing its conductivity. The deuterium in-diffusion was realized utilizing the RF remote plasma method and the profiles obtained by SIMS. The experimental conditions of deuteration studied were plasma power, sample temperature and hydrogenation duration. The results show that hydrogen can be introduced in the AlGaN/GaN HEMT structure at very high concentrations probably bonding to acceptor-like intrinsic defects and acceptor impurities. Although for the hydrogenation conditions attempted here, the hydrogen reached mainly the top layers; GaN, AlGaN and the AlGaN/GaN interface beneath which the two-dimensional electron gas lays. However, some hydrogen in-diffuses through the disordered core of the dislocations reaches very deep in the structure at constant concentration close to  $10^{16} \text{ cm}^{-3}$ .

<sup>3</sup>. The highest hydrogen concentration is obtained in the AlGa<sub>N</sub> layer at thin region parallel to the interface against which the TEG is confined. This high hydrogen concentration systematically found at the AlGa<sub>N</sub>/Ga<sub>N</sub> interface indicates a region rich in acceptor defects to which it bonds. The dose of in-diffused deuterium might be easily controlled over at least three orders of magnitude;  $10^{13}$  to  $10^{16}$  cm<sup>-3</sup> and depends mainly on the square of the plasma power and very lightly on the in-diffusing temperature.

From our results it can be concluded that the proper hydrogenation conditions to improve the charge transport properties of the HEMT structure are a plasma power around 10 Watts, a sample temperature close to 250°C and a hydrogenation time of 10 minutes. These results might open the possibility of improving the HEMT structure performance by just adding a simple and short hydrogenation step.

**Acknowledgments,**

The authors thanks M. en C. Ruben Huerta Cantillo for his technical assistance and A. S. Arreola-Pina acknowledges support by CONACYT of Mexico,

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