Effect of pH and structure on the channel conductivity of AlGaN/GaN heterostructure based sensors

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Abstract

We describe the pH dependence of the electron mobility as a function of various structural and electrolyte factors for unfunctionalised AlGa_N/Ga_N-based chemical sensors. The charge distribution across the sensor-electrolyte system is calculated self-consistently and the dependence of the Hall mobility of the two-dimensional electron gas on different scattering mechanisms is studied. Our calculations show that the pH of the electrolyte has a significant effect on the mobility and consequently the conductivity of the 2DEG channel electrons. A wide range of structures is examined to describe the correlation between the sensitivity and channel electron density. It is shown that the change of mobility with pH is a strong function of the structure of the sensor (AlGa_N, Ga_N-cap and oxide-layer thicknesses), while it is almost independent of the ionic strength of the electrolyte. The observed dependence of the Hall-mobility to the thickness of AlGa_N-barrier, Ga_N-cap and oxide layer can explain the discrepancy in the behaviour of the Hall-mobility, as reported by different groups.

Keywords: AlGa_N/Ga_N, oxide, mobility, conductivity, ISFET, pH,

1. Introduction

Since introduced by Bergveld,[1] Ion Sensitive Field Effect Transistors (ISFETs) have been studied extensively.[2-4] Although commercially available Si-based ISFETs can be found in many applications, noise and drift are still limiting factors for the realization of robust sensors.[5-7] The effects of the ionic concentration and pH of the electrolyte on the electronic transport parameters of different ISFETs has been reported for various materials, device configurations and applications. The effect of analytes on the carrier mobility of graphene-based biosensors has been investigated for various sensors for the detection of DNA,[8] cells,[9] bacteria,[10] pH, and protein.[11] It is also reported that the mobility of carriers in diamond-based biosensors is dramatically affected by the adsorption of analytes.[12-15] However, for the case of GaN-based chemical sensors, to our best knowledge, the effects of electrolyte pH and surface oxide thickness on carrier transport parameters have not been studied quantitatively. This paper presents results of a theoretical study of the effects of electrolyte pH on the electronic transport parameters of GaN-capped AlGaIn/GaN-based heterostructures designed for chemical sensing applications, including effects associated with native and/or deposited gallium oxide layers.

GaN belongs to the group III-N family of compound semiconductors, which is a relatively recent, but nonetheless now well-established material system in the field in optoelectronics and power electronics. The high mobility and high electron sheet densities that can be realized in III-N heterostructures, together with their relatively high sensitivity of the metal-group polar surfaces, makes III-N compounds an excellent material system for realizing sensors,[16] In addition, their chemical and thermal stability, non-toxicity and biocompatibility, make GaN-based materials an outstanding choice for realizing chemical and biochemical sensors. This is

particularly the case for sensors based on AlGaN/GaN field effect transistors which offer the same high gain combined with rugged durability that has made such structures so dominant in high power electronics.[17] GaN-based sensor technologies have been investigated extensively for gas sensors,[18-20] pH sensors,[16, 21] bio-chemical sensors[22-24] and ion sensors.[25-27] The GaN-based chemical sensors investigated via simulation in this work are based on actual structures for which ion sensing has previously been reported [25]: GaN-capped AlGaN/GaN heterostructures epitaxially grown by metal-organic chemical vapor deposition on a sapphire substrate, with an assumed native or thermally deposited gallium oxide layer. In the heterostructures studied, the top-surface layer is assumed to be covered with a layer of gallium oxide (see Fig. 1(a)) and no analyte-specific functionalization. Such a surface oxide layer is formed either unintentionally, through prolonged exposure to air or water, or intentionally as a relatively thick layer of crystalline oxide formed by thermal oxidation of the surface.[28] Gallium oxide is a transparent oxide with a wide energy band gap of 4.8 eV[29] which, owing to its material properties, is a promising semiconductor material for a wide range of applications from semiconducting lasers, UV detectors, and high temperature gas sensors, to water splitting,[30, 31] catalysis,[32, 33] and hydrogen detectors.[34-37]

The electronic transport properties of III-N semiconductors have been investigated extensively.[38-43] Even more extensively studied are the electronic transport properties of AlGaN/GaN heterostructures. The strong spontaneous and piezoelectric polarization in AlGaN/GaN heterostructures results in a high electric field which, coupled with the large conduction band discontinuity between AlGaN and GaN, leads to the formation of a quantum-confined electron accumulation layer at the heterointerface: a two-dimensional electron gas (2DEG).[44, 45] The 2DEG electron mobility in AlGaN/GaN heterostructures is an important

parameter often used to assess the epitaxial quality and to optimize the performance of high electron mobility transistors (HEMTs). Over the past few years, both experimental [46-48] and theoretical[39, 47, 49-56] efforts have provided significant insight into the transport properties of 2DEGs in AlGaIn/GaN-based heterojunctions. The electron mobility in such heterojunctions is limited by intrinsic and extrinsic scattering mechanisms: extrinsic scattering being associated with intentional and/or unintentional impurities in the GaN and AlGaIn layers, and interface-roughness, whereas intrinsic scattering being associated with fundamental mechanisms, such as polar-optical phonon scattering, that are inherent to the nature of the material.

For the case of chemical sensors based on AlGaIn/GaN heterostructures, the chemical environment of interest interacts with the "ungated" surface potential which then modulates the electronic transport parameters of the 2DEG channel. Hence, sensor performance optimization requires detailed insight into how 2DEG transport parameters are affected by heterostructure design and, importantly, the specific nature of the ungated surface which must needs include the presence of unavoidable native oxide. While some experiments suggest that the mobility of the channel increases with the deposition of aluminium oxide (Al_2O_3),[57, 58] others have reported the opposite trend.[59, 60] Other reports have also shown that the thickness of the GaN-cap and the AlGaIn barrier can cause the mobility of the 2DEG to increase or decrease depending to the specific epitaxial structure of the sensor. It must be noted, however, that in spite of reported studies^[30, 31, 61], oxide-electrolyte interactions in GaN-based sensors are not well understood, and that additional studies are required to gain insight in to the effect of such surface oxides on the electronic transport properties of the 2DEG channel, which determine ultimate sensitivity of any GaN-based chemical sensor, including effects associated with oxide thickness and its crystallinity, as well as the nature of the electrolyte to which the surface is exposed.

In what follows, the paper is divided into two additional sections. Firstly, the theoretical framework employed in this work for the calculation of 2DEG transport parameters in an electrolyte solution is presented. This is followed by presentation of results and discussion on the dependence of the total 2DEG mobility on the various scattering mechanisms as a function of pH, ionic strength and the epitaxial structure of a GaN-based sensor.

2. Theoretical framework

When a semiconductor is placed in an electrolyte, the space-charge region redistributes on both sides of the interface. Electrons move across the interface until their chemical potential is balanced by band bending at the surface of the semiconductor. Due to adsorption and desorption of ions and counter-ions at the surface, a triple-layer[62] will form on the electrolyte side which will also contribute to an additional potential drop in the semiconductor. The surface charging mechanism and the binding of the electrolyte ions are modelled based on the theory developed by Sverjensky et al.[62-66] According to the triple-layer model (TLM), protons and hydroxide ions adsorb directly to the surface of the oxide (O-plane), resulting in a surface sheet charge density σ_0 (Cm^{-2}), while the ions, M^+ and L^- of the 1:1 electrolyte/salt adsorb at the closest distance β to the surface (β -plane), resulting in a sheet charge density σ_β (Cm^{-2}). As a result, the charged species in both solid and electrolyte redistribute themselves to keep the system charge-neutral. Redistribution of the counter-ions in the electrolyte forms a diffuse layer at the closest distance d to the surface. Schematics of the device and the corresponding band structure are depicted in Figure 1.

According to the theory developed by Gordon et al.,[67] the density of the occupied states at the interface between the GaN-cap and the surface oxide (native or annealed) determines the effective barrier height between the oxide and the GaN-cap and the corresponding electron density in the channel (2DEG). The experimental values for the interfacial trap densities as a function of the thickness of the oxide were used to interpolate the trap density at the oxide thicknesses of interest,[68-71] and the obtained trap densities were then used to calculate the barrier height self consistently at the pH of the pristine-point-of-zero-charge (PPZC). The band offsets of the surface oxide with the GaN-cap and electrolyte and other important details of the model can be found in our previous work.[72] Finally, the Poisson-Boltzmann and Schrodinger equations were solved self consistently to obtain the charge distribution across the sensor and electrolyte.

The studied GaN-based structures are intended to serve as chemical sensors in the electrolyte. Therefore, all the mobility studies were performed at room temperature. For temperatures above 80 K, the electron mobility of the channel is limited by inelastic polar optical phonon scattering.[51] In this regime, a closed form does not exist for the inelastic processes, hence the linearized Boltzmann equation (LBE) must be solved directly.[53, 73-75] The effect of scattering mechanisms due to interface roughness, dislocation, piezoelectric, deformation potential and coulombic scattering were accounted for in the Ritz iteration of LBE.[47, 51, 54, 76, 77] Finally, the perturbation due to each subband was used to obtain the overall perturbation that in turn is used to calculate the Hall mobility.[50, 53] All the material parameters that are used in this work are listed in Table 1.

Table I. physical parameters used in the computation.

Parameter	unit	value	Reference
Permittivity of GaN ϵ_b		10.4	[44]
Effective Bohr radius a_B	Å	32.9	[78]
LO phonon energy	meV	90.5	[51]
Piezoelectric constant h_{14}	V/m	4.28×10^9	[51]
Deformation potential a_c	eV	8.5	[51]
Elastic constant C_L	N/m ²	2.66×10^{11}	[51]
C_T	N/m ²	0.62×10^{11}	[51]
Lattice spacing in the (0001) direction of wurtzite GaN c_0	Å	5.185	[79]
Dislocation density N_{Diss}	cm ⁻²	1×10^9	[54]
RMS height of the amplitude of the roughness Δ	nm	0.1	[50]
correlation length of roughness L	nm	1.5	[50]
Fraction of filled states f		1	[54]
equilibrium reaction rates for the adsorption of KNO ₃ $K_{s,1}$		4.81	[72]
$K_{s,2}$		10.91	[72]
K_{s,L^-}		2.661	[72]
K_{s,M^+}		2.658	[72]
Closets distance of the first and second layer of water β	nm	2.65	[72]
d	nm	5.43	[72]
Number of reactive surface sites N_s	site/nm ²	9.28	[72]

3. Results and discussion

For transport in quantum confined electron channels, such as in HEMTs and quantum-wells, LO-polar phonon emission is the mobility limiting energy relaxation mechanism at room temperature[47, 51, 53, 77] Figure 2.a shows the influence of electrolyte pH on the conduction band edge at the surface, and redox levels of water with respect to the Fermi level in a chemical sensor with a top layer structure defined by 20nm AlGaIn/ 1nm GaN-cap and 1 nm Ga₂O₃. These characteristics were calculated for a sensor at 300 K, with the surface exposed to 10^{-4} mol/L KNO₃/H₂O solution and KCl or HNO₃ (depending on the pH); the Al mole fraction x of the AlGaIn barrier layer is $x = 0.3$. The effect of electrolyte pH on the energy locations E_i of the i -th ($i=1, 2, 3$, and 4) subband of the 2DEG with respect to the Fermi level are depicted in Figure 2.b. For the various epitaxial structures and pH levels shown in Figure 2.b, the minimum calculated

energy difference between ground state (subband E_1) and the next occupied sub-band E_2 is 117.95 meV, which is greater than the optical phonon energy of GaN (87.3 meV). Hence, for the conditions depicted in Figure 2.b, optical phonon emission scattering fundamentally limits 2DEG electron mobility. The effect of the pH and thickness of the top epitaxial layers in the structure (manifested as changes in N_s) for various top layer epitaxial layer thicknesses when limited by individual scattering mechanisms of deformation potential, dislocation density, piezoelectric phonon, interface roughness, and coulomb-scattering limited mobility by remote interfacial-charges at the GaN-cap/oxide interface are given in the supplementary material.

The calculated total 2DEG Hall mobility in the AlGaN/GaN-based sensor is shown in Figure 3.a as a function of the channel electron density N_s , where N_s is modulated by changes in pH as well as by thickness of top layers in the sensor structure. Although the modulation of N_s is via circumstances unique to the sensing application (i.e. pH), the N_s - μ relationship follows the well-known behavior reported in other studies, with the total mobility dominated by polar optical phonon scattering (Figure 3.b).[51, 52] For example, for a sensor with AlGaN/GaN-cap/Ga₂O₃ thicknesses in nm of 20/1/1, with a 2DEG sheet density and mobility near the vertex point in the N_s - μ characteristics, a change in the pH of the electrolyte from 2 to 12 induces a corresponding decrease in sheet density from $7.32 \times 10^{12} \text{ cm}^{-2}$ to $5.9 \times 10^{12} \text{ cm}^{-2}$ whilst the mobility increases from $1546 \text{ cm}^2/\text{Vs}$ at pH=2 to $1559 \text{ cm}^2/\text{Vs}$ at pH=6, and then decreases to $1516 \text{ cm}^2/\text{Vs}$ at pH=12. In contrast, a sensor formed using AlGaN/GaN-cap/Ga₂O₃ thicknesses of 30/1/1 nm,

which is in the N_s - μ regime in which the mobility decreases monotonically with increasing carrier concentration, a change in the pH of the electrolyte from 2 to 12 causes a corresponding decrease in 2DEG sheet density from $8.92 \times 10^{12} \text{ cm}^{-2}$ to $7.93 \times 10^{12} \text{ cm}^{-2}$ while the 2DEG mobility increases from $1429 \text{ cm}^2/\text{V.s}$ at pH=2 and to $1214 \text{ cm}^2/\text{V.s}$ at pH=12. Conversely, the latter trend is reversed in a sensor designed to operate in N_s - μ regime in which the mobility increases monotonically with increasing carrier concentration (as can be seen in Figure 3 for a sensor with AlGaIn/GaN-cap/Ga₂O₃ thicknesses of 15/1/1 nm).

From the preceding observations it follows that the sensitivity of a AlGaIn/GaN-based chemical sensor, operated on the basis of conductivity, is critically defined by the 2DEG N_s - μ characteristics of the sensor structure. This conclusion is consistent with the calculated 2DEG channel mobility and conductivity versus pH diagrams that are depicted in Figure 3.c and 3.d, respectively. The sensitivity on the basis of conductivity is defined as:

$$\frac{\partial \delta}{\partial \text{pH}} = q \left(n \frac{\partial \mu}{\partial \text{pH}} + \mu \frac{\partial n}{\partial \text{pH}} \right) \quad (1)$$

where the electron conductivity is $\delta = nq\mu$. Therefore, the lowest sensitivity corresponds to the regime in which the mobility decreases as the carrier concentration increases (e.g., with decreasing electrolyte pH). Such a low sensitivity corresponds to the response of a device that is biased on the right-hand side of the vertex point of mobility-concentration characteristics where $\frac{\partial \mu}{\partial \text{pH}} < 0$ and $\frac{\partial n}{\partial \text{pH}} > 0$, while the mobility of a device that is biased on the left-hand side of the vertex point would have the highest sensitivity to pH where $\frac{\partial \mu}{\partial \text{pH}} > 0$ and $\frac{\partial n}{\partial \text{pH}} > 0$. This finding can be used to optimize the sensitivity of the sensor, by shifting the response of the sensor to the left-hand side of the total-mobility versus N_s . This can be achieved by applying an electrical bias

to the electrolyte "gate" (i.e., in reference electrode configuration), by optimizing the epitaxial structure and/or doping of the sensor (such as by changing the thickness or Al mole fraction of the AlGaN barrier region).

Figure 4 depicts the changes in 2DEG mobility of a sensor versus electrolyte ionic strength. The calculation is performed for pH corresponding to the pristine-point-of-zero-charge (PPZC) of the sensor surface, so that the effect of the pH on the surface charge is minimized. The calculations demonstrate that, in this case, the mobility is not significantly dependent on ionic strength at the PPZC of the sensor.

The above presented results and discussion provide significant insight that may enable elucidation of reported non-idealities in GaN-based chemical sensors. The study performed by Podolska et al., employing an AlGaN/GaN heterostructure sensor with no GaN-cap, showed a U-shape response of the 2DEG channel resistance to pH [81, 82]. The observation of such a response suggests that the surface can become highly protonated at low pH values, thus causing a significant modulation in 2DEG sheet density, effectively shifting the bias-point of the device from moderate N_s values to very high N_s , and passing through the vertex point of the N_s - μ characteristics.

Regarding the influence of the epitaxial structure of the sensor on the electronic transport properties and sensitivity of an AlGaN/GaN heterostructure sensor, the N_s - μ characteristics of the 2DEG can be used to characterize the dependence of the transport parameters on the

thickness of the AlGaIn-barrier, GaN-cap and oxide layer. Figure 5.a shows that under exposure to electrolyte the electron sheet density in the channel is sensitive to, in descending order of influence, the thickness of the AlGaIn barrier, the GaN-cap and the oxide layer. However, the relative changes of the electron Hall mobility, shown in Figure 5.b, are more complicated.

The effect of variation of thickness of the AlGaIn barrier has been widely studied and the results shown in Figure 5 for a sensor structure in ionic solution are consistent with the literature for any (non-sensor) AlGaIn/GaN heterostructure. When the thickness of the AlGaIn increases from 10 to 20 nm, the calculated electron density and the corresponding mobility increase. In contrast, when the thickness of the AlGaIn increases from 20 to 30 nm, the calculated electron density increases, while the mobility decreases. Heikman et al. reported that increasing the thickness of an $\text{Al}_{0.32}\text{Ga}_{0.68}\text{N}$ barrier from 5 to 7.5nm increases the sheet electron density from 0.2×10^{13} to $1.5 \times 10^{13} \text{ cm}^{-2}$, with the mobility increasing from 900 to 1700 $\text{cm}^2/\text{V.s}$, however when the thickness of the AlGaIn barrier is increased beyond 10 nm the mobility decreases.[83] The theoretical study reported by Zhou et al. for Al_2O_3 -capped structures shows the increase of the thickness of the AlGaIn barrier and its corresponding fixed charges enhances the mobility within a certain range.[58]

In contrast to the AlGaIn layer thickness effects, even a thin GaN-cap layer leads to an increase in the electric field strength of the AlGaIn-barrier and lowering of the barrier height at the GaN-cap/oxide interface, and consequently the channel electron density decreases with increasing thickness of the GaN cap-layer.[72, 84] When the thickness of the GaN-cap increases from 0.3 to 8 nm for an AlGaIn-barrier thickness of 20 nm, the calculated electron density decreases, with a corresponding decrease in mobility. However, when the thickness of the AlGaIn-barrier is increased to 25 nm, and the thickness of the GaN-cap from 1 to 8 nm, the sheet electron density

decreases, with the mobility increasing. Hence, for a sensor structure design with an electron density below the sheet density at which the maximum mobility is reached in the N_s - μ characteristics, an increase in the thickness of the AlGaIn-barrier or a decrease in the thickness of the GaN-cap results in an increase electron density and an increase in the mobility. However, if the heterostructure design yields an electron density that exceeds the sheet density corresponding to the vertex of the N_s - μ characteristics (this can differ significantly from one practical device to another), the mobility of the channel decreases. These observations suggest that the heterostructure design has a direct impact on electronic transport parameters which, for chemical sensors, strongly influence device sensitivity and response. Again the above observations are consistent with reported experimental results: Kordos et al. reported that an extra 3 nm GaN-cap layer on an undoped 25 nm AlGaIn barrier decreased the sheet carrier density from 0.95×10^{13} to $0.81 \times 10^{13} \text{ cm}^{-2}$, while the mobility increased from 1410 to 1840 $\text{cm}^2/\text{V.s}$. [85] Heikman et al showed that an increase of the thickness of the GaN-cap from zero to 25 nm for a GaN/AlGaIn/GaN heterostructures with a fixed AlGaIn thickness of 20 nm, corresponds to a decrease in the sheet electron density from 1.3×10^{13} to $0.7 \times 10^{13} \text{ cm}^{-2}$, while the mobility increases from 1300 to 1800 $\text{cm}^2/\text{V.s}$ when the thickness of the cap is 10nm, followed by a decrease to 1600 $\text{cm}^2/\text{V.s}$ when the thickness of the GaN-cap reaches 25 nm. [83] A theoretical study performed by Asgari et al. reproduced these experimental results by fitting the doping density of the AlGaIn-barrier. [86]

Since chemical sensor response and sensitivity is influenced by the 2DEG electronic transport parameters, it is important to take into account the effects of the thickness of the oxide layer, for which limited understanding exists in the literature. In this work the calculated 2DEG sheet

density and mobilities are presented for specific AlGaIn/GaN heterostructure-based sensors that have been used in practice. However in general, and within the theoretical framework employed in this work, it is noted that an increase in the oxide layer thickness results in a slight decrease in the sheet electron density of the channel, and that oxide thickness effects on 2DEG mobility arise indirectly as a consequence of modulation of the 2DEG density and are thus determined by the N_s - μ characteristics of the heterostructure. It is important to note that since the changes in mobility induced by native and/or deposited oxides are dictated by the N_s - μ characteristics of the heterostructure design, including extrinsic effect associated with crystal growth quality, these observations helps clarify apparently contradicting published experimental results. For example, in their study of the effect of Al_2O_3 deposition on GaN-based transistor structures, Ye et al. observed that that oxide deposition results in increased 2DEG mobility.[57] Zhou et al. reported that post-oxide deposition annealing increased 2DEG mobility by 40% at room temperature.[87] In contrast, Liu et al. reported that formation of AlO_x via immersion in H_2O_2 , on AlGaIn/GaN structures without GaN-cap layer, resulted in an increase in sheet density with a concomitant decrease in 2DEG .[59] Similar observations were reported by Basu et al.[60] and Lee et al.[88] for Al_2O_3 deposited or grown using different methods. It is important to note that while the 2DEG concentration-mobility are in agreement to the above presented discussion, the reported observation of an increase in 2DEG sheet density with oxide thickness suggests that a more complex model for the native and/or deposited oxides on AlGaIn/GaN-based sensor structures necessitates the inclusion of all native oxide and GaN-cap/oxide interface charges. The development of such comprehensive model, however, is hampered by the lack of knowledge on the density and energy levels of oxide defects and interface states.

4. Summary and conclusion

In this work the effect of various electrolyte and structural parameters have been investigated for unfunctionalised AlGaIn/GaN transistor-based chemical sensors. Calculations have shown that for such sensors the pH of the electrolyte has a significant effect on the mobility and consequently the conductivity of the 2DEG channel electrons. The rate of change of mobility as a function of channel electron density becomes much higher as the channel electron density goes beyond the vertex point of the N_s - μ diagram. It was also shown that a device that is biased on the left-hand side (low electron sheet density) and right-hand side (high electron sheet density) of the vertex of the N_s - μ diagram, would have the highest and lowest sensitivity in terms of conduction to the pH. In practice, this finding can be used to design chemical sensors with higher sensitivity to pH and a wide measurement range. The changes of mobility with the ionic strength are not as significant compared to the changes of mobility with pH, which can be attributed to the relative changes of the conduction band edge and the corresponding change of channel-electron density. It was also suggested that the relative changes of mobility with pH can be a contributing factor to the unexpected behaviour of some devices. With respect to device structure, the calculations predict the changes of mobility with respect to changes of the thickness of the AlGaIn-barrier, GaN-cap and the oxide to a good proximity, as matched to other studies. In summary, our model could explain the discrepancy in the behaviour of the Hall-mobility of the 2DEG channel as a function of the thickness of the AlGaIn-barrier, GaN-cap and oxide layer, as reported by different groups. Our calculations can also predict the sensitivity of the mobility of the GaN-based chemical sensors to the pH and structure of the sensor. These findings can be used to optimize the response of the device for a particular application.

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a)

b)

Figure 1. (a) Schematic diagram of a typical Ga-polar AlGaIn/GaN-based chemical sensor. The GaN-buffer is unintentionally doped (UID) (b) calculated band diagram when the surface is exposed to a 10^{-1} mol/L $\text{KNO}_3/\text{H}_2\text{O}$ solution with $\text{pH} = 12$. The black, blue and red lines correspond to the energy levels of interest (conduction and valence bands and redox levels of water), Fermi level, and channel electron density (cm^{-3}) respectively. Triple-layer refers to the specific distribution of adsorbed liquid-molecules next to the surface.

a)

b)

Figure 2. (a) Relative changes of the conduction band edge for a sensor with top layer structure defined by AlGaIn/GaN-cap/Ga₂O₃ (20/1/1 nm) when exposed to a solution of 10^{-1} mol/L $\text{KNO}_3/\text{H}_2\text{O}$ as a function of pH, showing also the redox levels of water. (b) Variation in the energy position of the 2DEG sub-bands E_i for $i=1, 2, 3$, and 4 with respect to the Fermi level as a function of 2DEG sheet density N_s . Here, N_s is modulated by changes in the pH of the

electrolyte (10^{-4} mol/L $\text{KNO}_3/\text{H}_2\text{O}$ and KCl or HNO_3) and also by the design of the three top most layers of the sensor's epitaxial structure. The symbols $\diamond$, $\circ$, $\times$, $\square$, Δ , and $\diamond$, correspond to AlGaIn/GaN-cap/Ga₂O₃ thickness in nm of 15/1/1, 20/1/1, 20/4/1, 20/8/1, 25/1/1 and 30/1/1, respectively. For each presented structure, the symbols from left to right correspond to the changes of pH from 2 to 12.

Figure 3. Calculated (a) total mobility and (b) mobility limited by polar longitudinal-optical phonon scattering as a function of N_s as varied by the changes in pH (surface is exposed to 10^{-4} mol/L $\text{KNO}_3/\text{H}_2\text{O}$ and KCl or HNO_3) and thickness of various layers of the structure. Calculated (c) total mobility and (b) conductivity as a function of pH. Symbols $\diamond$, $\circ$, $\times$, $\square$, Δ , $\diamond$, correspond to AlGaIn/GaN/Ga₂O₃ thickness in nm of 15/1/1, 20/1/1, 20/4/1, 20/8/1, 25/1/1 and 30/1/1, respectively.

Figure 4. Ionic strength dependence of the total mobility (a) and conductivity (b) for GaN-based chemical sensor with AlGaIn/GaN/Ga₂O₃ thickness of 20/1/1 nm when the surface is exposed to 10^{-4} mol/L KNO₃/H₂O solution at pH=pH_{ppzc}.

Figure 5. (a) Calculated electron density and (b) total mobility of the channel as a function of the thickness of the oxide, GaN-cap and AlGaIn-barrier when the surface is exposed to 10^{-4} mol/L KNO₃/H₂O solution at pH=pH_{ppzc}. The thickness of the epitaxial layers (AlGaIn/GaN-cap/oxide) is represented by: ($\diamond$ -1-1), (20- $\circ$ -1), (25- $\triangle$ -1), (20-4- $\square$), (25-1- $\times$), respectively. The cases considered follow practical sensor design values.