

# Surface State Spectrum of AlGa<sub>N</sub>/AlN/GaN Extracted from Static Equilibrium Electrostatics

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**Abstract**—We extract an AlGa<sub>N</sub> surface state spectrum with a density ( $D_{SS}$ ) ranging between  $1.4 \times 10^{12}$  and  $4.7 \times 10^{12}$   $\text{eV}^{-1}\text{cm}^{-2}$ . The low  $D_{SS}$  is achieved with *in-situ* SiN passivation. The  $D_{SS}$  are extracted from ungated AlGa<sub>N</sub>/AlN/GaN heterostructures with varied AlN thicknesses between 0 to 2 nm: Increased AlN thicknesses in heterostructures monotonously increase 2DEG densities  $N_{sh}$  and AlGa<sub>N</sub> surface potential energies  $q\phi_s$ , and the  $D_{SS}$  is extracted with  $\Delta N_{sh}-\Delta\phi_s$  correlations. The  $D_{SS}$  extraction methodology in this work features calibrated polarization charge values, Hartree approximation based 2DEG profile calculation, and incorporated C-GaN substrate impact on 2DEG. We also extract the charge neutrality level at the AlGa<sub>N</sub> surface, which is  $\sim 0.95$  eV below conduction band minimum.

**Index Terms**—AlGa<sub>N</sub> surface state, III-N HEMT, polarization charge, 2DEG quantum well,

## I. INTRODUCTION

ALGAN/GAN high electron mobility transistors (HEMTs) featuring a high current density and a high breakdown voltage are promising candidate devices in power electronics and 5G/6G RF applications [1]–[4]. High AlGa<sub>N</sub> surface state density ( $D_{SS}$ , in  $\text{eV}^{-1}\text{cm}^{-2}$ ) has been a major problem that compromises efficiency of AlGa<sub>N</sub>/GaN HEMTs. High  $D_{SS}$  causes current collapses [5], induces high gate leakage [6], and reduces breakdown voltage [7] of HEMTs. To reduce the AlGa<sub>N</sub>  $D_{SS}$ , passivation solutions have been explored [8]–[10].

Quantitative evaluation of AlGa<sub>N</sub> surface passivation solutions relies on accurate measurement of the  $D_{SS}$ .  $D_{SS}$  characterization methods are multiple, but they can be simply categorized into dynamic and static methods depending on usage of bias voltages. In dynamic methods, multiple bias voltages—direct current (dc) or alternating current (ac) signals—are applied on metal/insulator/AlGa<sub>N</sub>/GaN MIS capacitors or MIS-HEMT devices, and the  $D_{SS}$  is extracted from surface state capture/emission responses. The accuracy of dynamic methods is challenged by correct determination of the steady state response and of the equivalent circuit of the test structures. This challenge is especially problematic for III-N heterostructures because of their multiple barriers/interfaces and usual lack of fast-responding dopants. In contrast, in static equilibrium methods for  $D_{SS}$  extraction, near-zero biases are

applied, and the electrostatics of heterostructures thus remain unvaried. In these methods, ungated heterostructures are fabricated with multiple AlGa<sub>N</sub> (or InAlN) barrier or AlN interlayer (IL) thicknesses, and the  $D_{SS}$  is extracted by correlating variations of 2DEG sheet densities ( $N_{sh}$ , in  $\text{cm}^{-2}$ ) with those of barrier surface potential energies ( $q\phi_s$ ,  $q$  is elementary charge) [11]–[17]. The static methods are based on electrostatics at rigorously equilibrium states; the surface states within  $q\phi_s$  intervals are thoroughly counted. So far, the  $D_{SS}$  reported with static methods are generally high [11]–[17]: the lowest reported  $D_{SS}$  of the AlGa<sub>N</sub> is  $4.6 \times 10^{12}$   $\text{eV}^{-1}\text{cm}^{-2}$  in [13] with optimized surface etching [12].

Accurate calculation of the electrostatics of heterostructures is crucial to static methods. In this work, we demonstrate a fully analytical static method featuring (a) Hartree approximation based 2DEG profile calculation, (b) inclusion of the substrate impact on the  $N_{sh}$ , and (c) experimental calibration of polarization charges ( $\sigma$ , in  $\text{C}/\text{cm}^2$ ) of the heterostructure interfaces. We extract a low- $D_{SS}$  spectrum with an average magnitude of  $\sim 2.9 \times 10^{12}$   $\text{eV}^{-1}\text{cm}^{-2}$ , demonstrating successful AlGa<sub>N</sub> surface passivation by an *in-situ* SiN. To our knowledge, the  $D_{SS}$  is the lowest compared to past studies using static methods [11]–[17]. Also, it is the first time that a surface state spectrum is extracted using a static method, attributed to consistent  $\phi_s-N_{sh}$  correlations among the heterostructures in this study. In addition, we extract the charge neutrality level of the SiN passivated AlGa<sub>N</sub> surface, which is  $\sim 0.95$  eV below AlGa<sub>N</sub> conduction band  $E_C$  minimum.

## II. EXPERIMENTAL

Epitaxial structures were grown by MOCVD on high-resistivity 200 mm Si (111) substrates using the method in [18], [19]. A schematic of top layers of samples in this work is shown in Fig. 1a. 300 nm undoped GaN (i-GaN) was grown on a thick C doped GaN layer (C-GaN) [20]. The fully relaxed i-GaN provides a template for pseudomorphic growth of the AlGa<sub>N</sub>/AlN layers. Two sets of samples with varied epitaxial AlN/Al<sub>0.25</sub>Ga<sub>0.75</sub>N thicknesses were prepared: one set is composed of a 0, 0.5, 1, 1.5, or 2 nm AlN IL and a 15 nm AlGa<sub>N</sub> barrier; the other set of a 1 nm AlN and a 4, 10, or 15 nm AlGa<sub>N</sub>. The AlN/AlGa<sub>N</sub> layers were undoped. The AlGa<sub>N</sub> surfaces of all samples were passivated with *in-situ* SiN [21].

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The in-situ SiN growth method has been introduced in [22].  $250 \times 250 \mu\text{m}^2$  square Van der Pauw (VDP) structures were fabricated for measurement of 2DEG  $N_{\text{sh}}$  and sheet resistances ( $R_{\text{sh}}$ ). The  $N_{\text{sh}}$  was obtained from Hall effect measurements of VDP structures. HEMTs with  $1 \mu\text{m}$  gate length and  $10 \mu\text{m}$  width were fabricated for threshold voltage ( $V_{\text{th}}$ ) measurement. In the gate region of HEMTs, the SiN layer was etched, and TiN was deposited on AlGaIn as the gate metal [21].  $V_{\text{th}}$  of HEMTs was extracted with the linear extrapolation method [23] with a  $0.1 \text{ V}$  drain-to-source voltage.

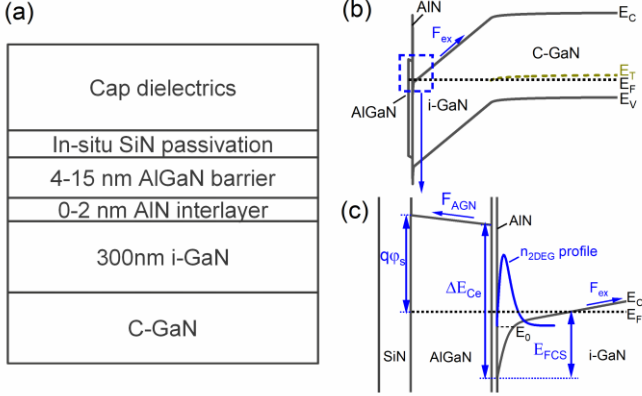


Fig. 1 (a) Schematic layer information of the heterostructure near GaN surface. (b) Schematic energy band diagram of AlGaIn/AlN/i-GaN/C-GaN. (c) Zoom of the region near GaN surface with simulated 2DEG concentration  $n_{\text{2DEG}}$  distribution.

### III. RESULTS, MODELING, AND DISCUSSION

The 2DEG  $R_{\text{sh}}$  and  $N_{\text{sh}}$  as functions of the AlN IL thickness ( $t_{\text{AN}}$ ) and the AlGaIn barrier thickness ( $t_{\text{AGN}}$ ) are shown in Fig. 2. In Fig. 2a, we observe that the  $N_{\text{sh}}$  increases monotonously with the  $t_{\text{AN}}$ , but the  $R_{\text{sh}}$  reaches the lowest with a  $t_{\text{AN}}$  of  $0.5 \text{ nm}$  or  $1 \text{ nm}$ . A thin AlN IL is known to push 2DEG centroid away from the AlGaIn/GaN interface and reduces interface scattering and AlGaIn alloy disorder scattering of the 2DEG [24]. This should improve the 2DEG mobility. As for the degraded 2DEG mobility with the  $1.5 \text{ nm}$  or  $2 \text{ nm}$  AlN IL, it may result from increased scattering from the AlN/GaN interface roughness or misfit dislocations in the AlN/AlGaIn. Because the tensile stress built within the AlN/AlGaIn on a relaxed GaN substrate increases with their thicknesses. Our activities are still ongoing to fully understand the mechanism behind the 2DEG mobility of various heterostructures. Note that all  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  layers in this work are still below their critical thicknesses of strain relaxation [25]. In later discussion, we will also show how the strain status of the AlGaIn and the AlN is examined with  $V_{\text{th}}-t_{\text{A(G)N}}$  curves.

We apply the  $N_{\text{sh}}-t_{\text{AN}}$  and  $N_{\text{sh}}-t_{\text{AGN}}$  dependences to this AlGaIn surface state study. Spontaneous polarization charge values ( $P_{\text{AGN}}^{\text{SP}}$ ) at c-plane surfaces of wurtzite  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  increase with Al content  $x$  [26], [27]. On relaxed GaN substrates, the tensile strain induced by lattice mismatch creates additional piezoelectric charges in the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  ( $P_{\text{AGN}}^{\text{PZ}}$ ), which also increases with  $x$ . Due to a much higher total polarization charge of  $\sigma_{\text{AN}}$  in the AlN IL ( $\sigma_{\text{AN}} = P_{\text{AN}}^{\text{SP}} + P_{\text{AN}}^{\text{PZ}}$ ) than the  $\sigma_{\text{AGN}}$  in the  $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$  barrier, the AlN IL increases the effective conduction band offset  $\Delta E_{\text{Ce}}$  between AlGaIn and GaN [24]. As a result, the AlN IL induces a positive shift of the AlGaIn surface potential energy  $q\Delta\phi_{\text{S}}$ . The positive  $q\Delta\phi_{\text{S}}$  makes the net

surface state charge ( $qN_{\text{SS}}$ , in  $\text{C}/\text{cm}^2$ ) more positive, resulting in increased  $N_{\text{sh}}$  of 2DEG to maintain charge neutrality. This means that, among samples with varied AlN IL thicknesses  $t_{\text{AN}}$ , variations of  $N_{\text{SS}}$  and  $N_{\text{sh}}$  compensate each other

$$\Delta N_{\text{SS}} = \Delta N_{\text{sh}} \quad (1)$$

The averaged  $D_{\text{SS}}$  in each  $q\Delta\phi_{\text{S}}$  is then

$$D_{\text{SS}} = \frac{\Delta N_{\text{SS}}}{q\Delta\phi_{\text{S}}} = \frac{\Delta N_{\text{sh}}}{q\Delta\phi_{\text{S}}} \quad (2)$$

The  $\Delta N_{\text{sh}}$  caused by  $t_{\text{AN}}$  variations are derived from Hall effect measurements in Fig. 2a. The remaining task for  $D_{\text{SS}}$  extraction with (2) is accurate calculation of  $\Delta\phi_{\text{S}}$ , which is explained hereafter.

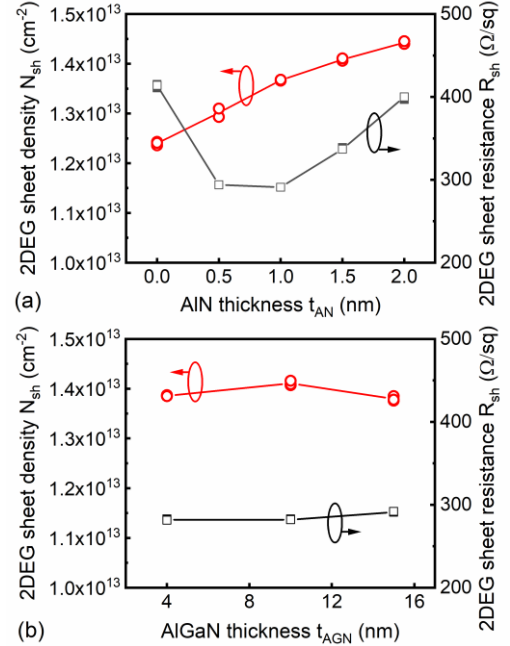


Fig. 2 2DEG  $N_{\text{sh}}$  and  $R_{\text{sh}}$  with varied (a)  $t_{\text{AN}}$  and (b)  $t_{\text{AGN}}$  in the heterostructure. The heterostructures in (a) with the same  $15 \text{ nm}$  AlGaIn; the samples in (b) with the same  $1 \text{ nm}$  AlN.

As the schematics illustrated in Fig. 1c, fundamentally, calculation of the  $\phi_{\text{S}}$  requires knowledge of (a) the  $N_{\text{sh}}$ , (b) the quantum well potential profile at GaN surface, and (c) the  $\sigma$  at heterostructures interfaces. The quantum well potential profile is required to establish the boundary potential energy for the AlGaIn/AlN, while the  $N_{\text{sh}}$  and the  $\sigma$  are required to calculate electric fields across the AlGaIn/AlN. The  $N_{\text{sh}}$  is obtained experimentally in Fig. 2. Next, we make particular efforts in improving accuracy of factors (b) and (c) compared to previous works [11]–[17].

We adopt the Hartree method to calculate the quantum well potential profile [28]. The Hartree approximation is advantageous over triangular well approximation by correctly considering electron-electron interaction in many-electron systems [28]. In the Hartree method, the impact of the external field  $F_{\text{ex}}$  on  $N_{\text{sh}}$  can be analytically incorporated [29]. As illustrated in Fig. 1b, the  $F_{\text{ex}}$  is built between the 2DEG quantum well edge and the C-GaN: in the degenerate quantum well at the i-GaN surface, the Fermi level  $E_f$  is above conduction band  $E_c$ ; in the C-GaN, the  $E_f$  is pinned in the lower half of band gap by ionized C acceptors [20]; a constant  $F_{\text{ex}}$  is thereby built in the undoped i-GaN layer. In the following analytical calculation for the quantum well potential profile, the electron-electron

interaction induced Hartree potential [28] and the  $F_{ex}$  induced external potential are both included.

As shown in Fig. 1c,  $E_{FCS}$  is the boundary potential energy at the GaN surface between the  $E_F$  and the  $E_C$ . In a 2DEG quantum well, the  $N_{sh}$  has the following dependence on the  $E_{FCS}$  [28]

$$N_{sh} = D_{GN} kT \ln \left[ 1 + \exp \left( \frac{E_{FCS} - E_0}{kT} \right) \right] \quad (3)$$

where  $k$  is the Boltzmann constant,  $T$  is temperature,  $E_0$  is the energy of the first sub-band in a quantum well with respect to  $E_C$ , and  $D_{GN}$  is the 2D density of states (DOS) in a GaN quantum well

$$D_{GN} = C \frac{m_{GN}^*}{\pi \hbar^2} \quad (4)$$

where  $\hbar$  is the reduced Planck constant,  $m_{GN}^*$  is the electron density of states effective mass in the  $E_C$  of GaN, and  $C=1.1$  is a correction factor for the DOS.  $C$  is introduced because only the first sub-band is considered in the Hartree approximation [28]. By simulating an AlGaIn/AlN/GaN heterostructure with a 1D Poisson-Schrodinger solver [30], we note that 88%~91% of the 2DEG is occupied by the first sub-band in the GaN quantum well when the  $N_{sh}$  varies between  $3 \times 10^{12}$  and  $2 \times 10^{13} \text{ cm}^{-2}$ . Therefore, the first sub-band is dominant, but neglecting the second and other upper sub-bands causes underestimation of DOS by ~10%.  $C=1.1$  is thus introduced in (4) to compensate the DOS underestimation in the Hartree method.

Then we incorporate the  $F_{ex}$  impact on the GaN surface quantum well into the Hartree approximation method [28]

$$E_0 = \frac{3}{2} \left[ \frac{(\hbar c)^2}{4m^*} \right]^{1/3} + \frac{c - 3qF_{ex}}{b} \quad (5)$$

where  $b$  and  $c$  are two intermediate variables

$$c = 3qF_{ex} + \frac{33q^2 N_{sh}}{32\varepsilon} \quad (6)$$

$$b = \left( \frac{4cm^*}{\hbar^2} \right)^{1/3} \quad (7)$$

With knowledge of the  $N_{sh}$  and the  $F_{ex}$ , (3)-(7) help derive the boundary  $E_{FCS}$  and the sub-band level  $E_0$ . The distribution of the 2DEG in a quantum well follows the normalized Fang—Howard wave function [28]

$$\psi(x) = \frac{b^{3/2}}{\sqrt{2}} x \exp \left( -\frac{1}{2} bx \right) \quad (8)$$

As illustrated in the schematics Fig. 1c, after deriving the  $E_{FCS}$ , the  $\varphi_s$  is simply

$$\varphi_s = (\Delta E_{Ce} - E_{FCS})/q + F_{AGN} t_{AGN} \quad (9)$$

where  $F_{AGN}$  is the electric field across the AlGaIn (direction see Fig. 1c)

$$F_{AGN} = \frac{\sigma_{AGN} - \sigma_{GN} - qN_{sh}}{\varepsilon} - F_{ex} \quad (10)$$

and  $\Delta E_{Ce}$  is the effective conduction band offset  $\Delta E_{Ce}$  between the AlGaIn and the GaN, which increases with the AlN thickness  $t_{AN}$

$$\begin{aligned} \Delta E_{Ce} &= \Delta \chi_e + qF_{AN} t_{AN} \\ &= \Delta \chi_e + q \left( \frac{\sigma_{AN} - \sigma_{GN} - qN_{sh}}{\varepsilon} - F_{ex} \right) t_{AN} \end{aligned} \quad (11)$$

where  $F_{AN}$  is the electric field across the AlN,  $\varepsilon$  is the dielectric constant of wurtzite  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  ( $\varepsilon$  is almost the same for  $0 \leq x \leq 1$ ),  $\sigma_{GN}$  is the (spontaneous) polarization charge of GaN, and  $\Delta \chi_e$  is the constant difference of the electron affinity between  $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$  and GaN [31].

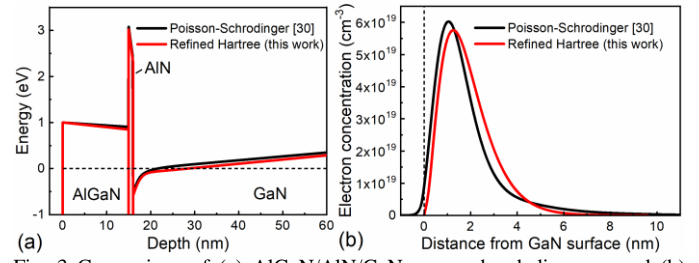


Fig. 3 Comparison of (a) AlGaIn/AlN/GaN energy band diagrams and (b) electron concentration distribution simulated by a Poisson-Schrodinger solver [30] and by the refined analytical Hartree method in this work. The same material parameters including a fixed  $\varphi_s$  of 1.0 eV are put in the two simulations. The simulated  $N_{sh}$  differences between the two methods remain lower than 1% when  $\varphi_s$  varies between 0.5 eV to 5 eV.

The analytical formula set (3)-(11) describes how a III-N heterostructure is simulated by a refined Hartree method. In Fig. 3, we verify resemblance of simulated energy band diagram and electron distribution with the refined Hartree method to those with the Poisson-Schrodinger solver [30]. The agreement is encouraging. The refined Hartree method achieves simple and analytical 2DEG simulation and  $\varphi_s$  calculation, which makes it a promising to be incorporated into future compact modeling.

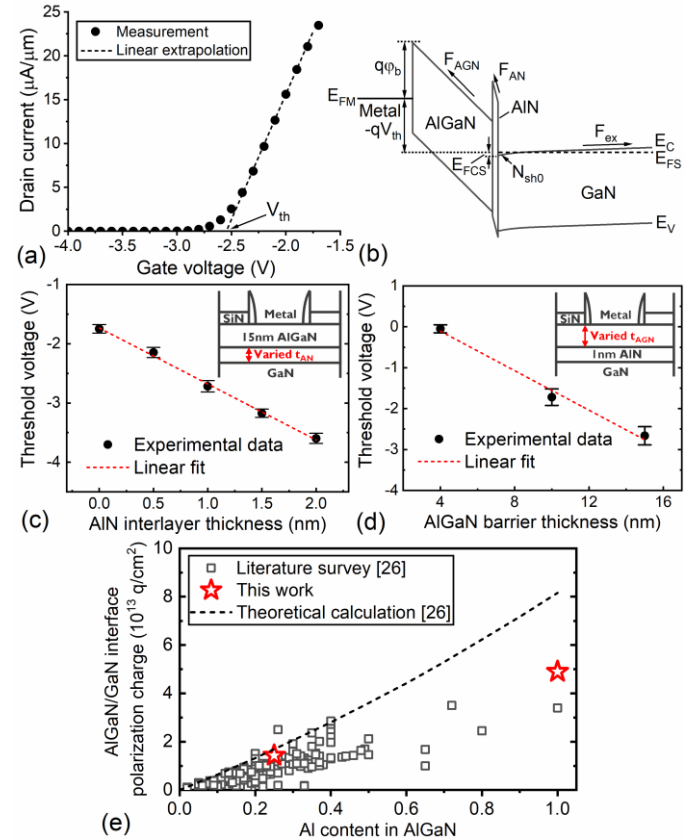


Fig. 4 (a) Illustration of  $V_{th}$  extraction from drain current-gate voltage curve at 0.1V drain to source voltage using linear extrapolation method. (b) Schematic of energy band diagram of HEMT gate region at  $V_{th}$ . (c) and (d) show  $V_{th}$  of HEMT as a function of  $t_{AN}$  or  $t_{AGN}$  with drain-to-source voltage of 0.1V; Insets show schematic device cross sections. (e) Extracted  $\sigma_{AN} - \sigma_{GN}$  and  $\sigma_{AGN} - \sigma_{GN}$  are compared to experimental data survey in literature and theoretical prediction by Dreyer *et al.* in [26].

(9)-(11) show how the  $\varphi_s$  depends on the  $\sigma$ . In previous studies [11]–[17], theoretical values of  $\sigma$  were adopted in  $\varphi_s$  calculation. But experimental  $\sigma$  usually deviate from theoretical

prediction [26], as shown in Fig. 4e. This necessitates applying experimentally calibrated  $\sigma$  into calculation of the  $\phi_S$ .

We extract the  $\sigma_{AN}-\sigma_{GN}$  and the  $\sigma_{AGN}-\sigma_{GN}$  from  $V_{th}-t_{A(G)N}$  correlations. As illustrated in Fig. 4a, The  $V_{th}$  of HEMTs is extracted with the linear extrapolation method on drain current-gate voltage curves [23]. As illustrated in Fig. 4b, the  $V_{th}$  of a HEMT is calculated by

$$V_{th} = \phi_b - F_{AGN}t_{AGN} - \frac{\Delta E_{Ce}}{q} + E_{FCS}(N_{sh0}) \quad (12)$$

where  $\phi_b$  is the gate Schottky barrier height,  $N_{sh0}$  is the remaining 2DEG density in the channel of HEMTs at  $V_{th}$ , approximately  $2 \times 10^{12} \text{ cm}^{-2}$ . Taking (10) and (11) into (12), we derive  $\Delta V_{th}$  vs  $\Delta t_{A(G)N}$

$$\begin{aligned} \Delta V_{th} &= -F_{AGN}\Delta t_{AGN} - F_{AN}\Delta t_{AN} \\ &= -\left(\frac{\sigma_{AGN} - \sigma_{GN} - qN_{sh0}}{\epsilon} - F_{ex}\right)\Delta t_{AGN} \\ &\quad -\left(\frac{\sigma_{AN} - \sigma_{GN} - qN_{sh0}}{\epsilon} - F_{ex}\right)\Delta t_{AN} \end{aligned} \quad (13)$$

(13) allows us to extract experimental  $\sigma_{AN}-\sigma_{GN}$  and  $\sigma_{AGN}-\sigma_{GN}$  from slopes of curves in Fig. 4c and 4d. The  $\sigma_{AN}$  and  $\sigma_{AGN}$  are lower than theoretical prediction, possibly due to partial strain relaxation of AlN and AlGaIn on the GaN substrate. The linearity of the  $V_{th}-t_{A(G)N}$  curves in (c) and (d) suggests that the tensile strain built within the AlGaIn and the AlN is consistent among all samples. The experimental  $\sigma$  are then fed into (8)-(10) for  $\phi_S$  calculation.

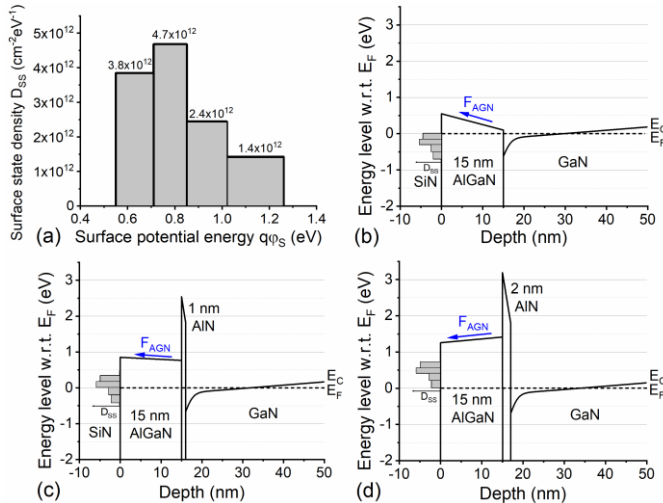


Fig. 5 (a)  $D_{SS}$  spectrum of AlGaIn surface as a function  $q\phi_S$ . Calculated energy band diagram of (b) SiN/15 nm AlGaIn/i-GaN/C-GaN, (c) SiN/15 nm AlGaIn/1 nm AlN/i-GaN/C-GaN, and (d) SiN/15 nm AlGaIn/2 nm AlN/i-GaN/C-GaN with  $D_{SS}$  distribution illustrated at AlGaIn surface. SiN, part of i-GaN, and C-GaN are not shown in (b)-(d) for simplicity.

The  $\Delta E_{Ce}$  increases substantially with the  $t_{AN}$ , as in (11), making  $\phi_S$  increase monotonously with  $t_{AN}$ . Five  $t_{AN}$  splits in this work create four  $\Delta\phi_S$  intervals. The  $D_{SS}$  in each  $\Delta\phi_S$  interval is calculated with (2) and shown in Fig. 5a. A  $D_{SS}$  spectrum is thus derived with a span of  $\sim 0.7\text{eV}$  and magnitudes varying between  $1.4 \times 10^{12}$  and  $4.7 \times 10^{12} \text{ eV}^{-1}\text{cm}^{-2}$ . The  $D_{SS}$  magnitudes within the spectrum indicate non-existence of discrete single states that have a surface density above  $1 \times 10^{12} \text{ cm}^{-2}$ . Besides the  $D_{SS}$ , complete energy band diagrams of the AlGaIn/AlN/GaN with varied AlGaIn/AlN thicknesses are also derived. Examples of the energy band diagrams are shown in Fig. 5b-d.

The energy band diagrams reflect electrostatics of the heterostructures at equilibrium. Interestingly, we can also derive the surface charge neutrality level  $E_{CNLS}$  of the AlGaIn from the energy band diagrams. The  $E_{CNLS}$  is practically defined as following: when the  $E_F$  overlaps with the  $E_{CNLS}$  at equilibrium, the net charge at the AlGaIn surface is zero. The  $E_{CNLS}$  of the AlGaIn represents a reference position of  $E_F$  at which the surface polarization charges are equally compensated by surface state charges. Among the energy band diagrams of Fig. 5b-d, a flip of the  $F_{AGN}$  direction is noted when the  $t_{AN}$  is varied between 0 nm and 2 nm. It means the polarity of the net surface charge is flipped, or in other words, the  $E_F$  sweeps over the  $E_{CNLS}$  of the AlGaIn. Based on the  $D_{SS}$  and the  $\phi_S$  with varied  $t_{AN}$ ,  $E_{CNLS}$  is estimated to be  $\sim 0.95 \text{ eV}$  below the  $E_C$  minimum of the AlGaIn surface. As shown in Fig. 5c, the AlGaIn is nearly flat-band with 1nm AlN, corresponding to a condition that the  $E_F$  is close to  $E_{CNLS}$ . In such conditions, varying AlGaIn thicknesses induces little  $\Delta\phi_S$ ; consequently, the  $N_{sh}$  and the  $R_{sh}$  of 2DEG vary little with the  $t_{AGN}$  in Fig. 2b. Knowledge of the  $D_{SS}$  and the  $E_{CNLS}$  correlates quantitatively the  $F_{AGN}$  with the  $\phi_S$  by

$$F_{AGN} = -\frac{qD_{SS}(q\phi_S - E_{CNLS})}{\epsilon} \quad (14)$$

Extension of the above relationship with (3)-(10) would enable prediction of the  $N_{sh}$  with given  $t_{AGN}$  and  $t_{AN}$  [32].

This work belongs to the  $D_{SS}$  extraction methods that make use of static equilibrium electrostatics of ungated heterostructures. In these methods,  $N_{sh}$  measurement and  $\phi_S$  calculation are the basic steps to derive the  $D_{SS}$ . Only small longitudinal fields are applied on VDP structures in the  $N_{sh}$  measurement, so the electrostatics of the heterostructures remain close to zero-bias conditions. In such near-zero-bias conditions, all defects comply with the same Fermi-Dirac distribution. This avoids complicated determination of the steady state and the equivalent circuit of test structures, which are usually error sources of  $D_{SS}$  in methods using dynamic bias voltages. Due to the methodology differences, the following discussion involves only the static equilibrium methods.

The fully analytical  $D_{SS}$  extraction methodology in this work features (a) experimentally calibrated  $\sigma$  of heterostructures and (b) Hartree approximation based 2DEG profile calculation. These are advances compared to traditional equilibrium electrostatics based  $D_{SS}$  extraction methods [11]–[17]. According to Fig. 4e and the equations (2) and (9)-(11), the use of theoretical  $\sigma$  values would usually result in overestimation of  $\sigma$ ,  $\phi_S$ , and  $\Delta\phi_S$ , and eventually underestimation of  $D_{SS}$ ; the  $D_{SS}$  underestimation degree would be approximately the same as that of the  $\sigma$  overestimation. As for the 2DEG profile calculation, we incorporate the substrate impact on 2DEG into the Hartree approximation method. This makes the methodology applicable to various substrates and is especially helpful for those studies with thin i-GaN channel layers.

It is worth noting that the  $D_{SS}$  reported with the static equilibrium methods were usually high, as summarized in Table I. This poses serious concerns, as a high  $D_{SS}$  of the barrier is a direct cause of degradation and reliability concerns—such as serious current collapses, high gate leakage, and low breakdown voltages—of HEMT or MIS-HEMT devices. In this work, the low  $D_{SS}$  of the AlGaIn and the high  $N_{sh}$  of 2DEG achieved with the *in-situ* SiN passivation are encouraging. It is

aligned with the good dc and RF performance demonstrated with our devices [4], [21]. The *in-situ* SiN reduces relaxation, cracking, and surface roughness of the AlGa<sub>N</sub> layer [22]. Moreover, it helps avoid AlGa<sub>N</sub> surface oxidation, which is a major cause of AlGa<sub>N</sub> surface states [33]. Since the *in-situ* SiN is not only critical for epitaxy engineering but also prevents air exposure of the AlGa<sub>N</sub>, it is found much superior to *ex-situ* SiN passivation [34].

TABLE I SUMMARY OF  $D_{SS}$  STUDIES THAT ARE BASED ON STATIC EQUILIBRIUM ELECTROSTATICS OF III-N HETEROSTRUCTURES

Ref.	Barrier	With AlN IL?	Method	Passivation/surface treatment	Avg. $D_{SS}$ ( $10^{12}$ eV <sup>-1</sup> cm <sup>-2</sup> )
[11]	Al <sub>0.34</sub> Ga <sub>0.66</sub> N	No	Vary $t_{AGN}$	w/o	>11
[13]	Al <sub>0.19</sub> Ga <sub>0.81</sub> N	No	Vary $t_{AGN}$	RIE <sup>a</sup>	4.6
[13]	Al <sub>0.24</sub> Ga <sub>0.76</sub> N	No	Vary $t_{AGN}$	RIE <sup>a</sup>	6.1
[13]	Al <sub>0.29</sub> Ga <sub>0.71</sub> N	No	Vary $t_{AGN}$	RIE <sup>a</sup>	7.5
[14]	Al <sub>0.3</sub> Ga <sub>0.7</sub> N	No	Vary $t_{AGN}$	w/o	7.8
[14]	Al <sub>0.3</sub> Ga <sub>0.7</sub> N	No	Vary $t_{AGN}$	SiN	17.8
[15]	Al <sub>0.35</sub> Ga <sub>0.65</sub> N Al <sub>0.4</sub> Ga <sub>0.6</sub> N	No	Vary Al% in AlGa <sub>N</sub>	SiN	18.5
[16]	In <sub>0.17</sub> Al <sub>0.83</sub> N In <sub>0.07</sub> Al <sub>0.93</sub> N	Yes	Vary $t_{IAN}$ <sup>b</sup>	N/A	35
[16]	In <sub>0.12</sub> Al <sub>0.88</sub> N In <sub>0.145</sub> Al <sub>0.855</sub> N	Yes	Vary Al% in InAlN	w/o	16.8
[17]	In <sub>0.169</sub> Al <sub>0.831</sub> N	No	Vary $t_{IAN}$	w/o	82.7
[17]	In <sub>0.182</sub> Al <sub>0.818</sub> N	No	Vary $t_{IAN}$	w/o	68.1
[17]	In <sub>0.098</sub> Al <sub>0.902</sub> N	No	Vary $t_{IAN}$	w/o	46.4
This work	Al <sub>0.25</sub> Ga <sub>0.75</sub> N	Yes	Vary $t_{AN}$	<i>In-situ</i> SiN	2.9

<sup>a</sup>RIE: Cl-based reactive ion etching [12]

<sup>b</sup> $t_{IAN}$ : InAlN thickness

Knowledge of the  $D_{SS}$  is not only important to evaluation of barrier passivation techniques, but also to modeling HEMT or MIS-HEMT. The extracted  $D_{SS}$  spectrum and the  $E_{CNLS}$  of the AlGa<sub>N</sub> make solid foundations for future compact modeling development: this includes modeling of access region resistances, gate/drain corner field distribution, gate leakage, current collapses, etc.

#### IV. CONCLUSIONS

In this work, we investigate surface state densities ( $D_{SS}$ ) of the AlGa<sub>N</sub>/AlN/GaN heterostructures passivated by the *in-situ* SiN. We demonstrate a fully analytical  $D_{SS}$  extraction method. In the method, we build quantitative correlations between the AlGa<sub>N</sub> surface states and the static equilibrium electrostatics of heterostructures with varied AlGa<sub>N</sub> barrier/AlN interlayer thicknesses. We introduce several key advancements that ensure accurate calculation of electrostatics: we apply the Hartree approximation method in quantum well potential profile calculation; we include analytically the C-GaN substrate impact on 2DEG distribution; and we calibrate experimentally polarization charge values of the III-N layers. With the optimized method, we report low  $D_{SS}$  varying between  $1.4 \times 10^{12}$  and  $4.7 \times 10^{12}$  eV<sup>-1</sup>cm<sup>-2</sup>, which proves successful AlGa<sub>N</sub> passivation with the *in-situ* SiN. Besides the  $D_{SS}$ , we also derive the charge neutrality level  $E_{CNLS}$  at the AlGa<sub>N</sub> surface, which is  $\sim 0.95$  eV below the  $E_C$  of the AlGa<sub>N</sub>. The fully analytical simulation method in this work is promising to be incorporated into future compact modeling, while knowledge of the  $D_{SS}$

spectrum and the  $E_{CNLS}$  will contribute to accurate trapping modeling in AlGa<sub>N</sub>/GaN (MIS-)HEMT.

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