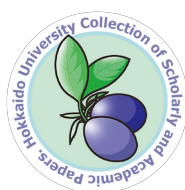




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Origin of positive fixed charge at insulator/AlGaIn interfaces and its control by AlGaIn composition

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Origin of positive fixed charge at insulator/AlGa_N interfaces and its control by AlGa_N composition

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The key feature for the precise tuning of V_{th} in GaN-based metal-insulator-semiconductor (MIS) high electron mobility transistors is the control of the positive fixed charge (Q_f) at the insulator/III-N interfaces, whose amount is often comparable to the negative surface polarization charge (Q_{pol}^-). In order to clarify the origin of Q_f , we carried out a comprehensive capacitance-voltage (C-V) characterization of SiO₂/Al_xGa_{1-x}N/GaN and SiN/Al_xGa_{1-x}N/GaN structures with Al composition (x) varying from 0.15 to 0.4. For both types of structures, we observed a significant V_{th} shift in C-V curves towards the positive gate voltage with increasing x . On the contrary, the Schottky gate structures exhibited V_{th} shift towards the more negative biases. From the numerical simulations of C-V curves using the Poisson's equation supported by the analytical calculations of V_{th} , we showed that the V_{th} shift in the examined MIS structures is due to a significant decrease in the positive Q_f with rising x . Finally, we examined this result with respect to various hypotheses developed in the literature to explain the origin of the positive Q_f at insulator/III-N interfaces. *Published by AIP Publishing.* [<http://dx.doi.org/10.1063/1.4986482>]

GaN-based metal-insulator-semiconductor high electron mobility transistors (MISHEMTs) become very attractive for applications in energy-efficient power switching devices.¹⁻¹⁰ However, achieving normally-off or enhancement mode transistors with the positive threshold voltage (V_{th}), which exhibit good performance, still remains a major challenge.² The key feature of the precise tuning of V_{th} in GaN-based MISHEMTs is the control of the positive fixed charge (Q_f) at the insulator/III-N interfaces.¹¹ The positive Q_f was reported for Al₂O₃/(Al, Ga)N,¹²⁻¹⁵ SiO₂/AlGa_N,¹⁵ and SiN/AlGa_N.^{16,17} Furthermore, it was well demonstrated by many groups that the amount of Q_f is often comparable to the negative polarization charge (Q_{pol}^-) at the insulator/III-N interfaces. In spite of that, the nature and location of Q_f is still not clear. To get a deep insight into this problem, we performed, in this report, a comprehensive capacitance-voltage (C-V) characterization of SiO₂/Al_xGa_{1-x}N/GaN and SiN/Al_xGa_{1-x}N/GaN metal-insulator-semiconductor (MIS) structures with Al composition (x) varying in a broad range, from 0.15 to 0.4. For both structures, we observed a significant V_{th} shift in C-V curves towards the positive voltage with increasing x . On the contrary, from the comparative measurements performed for the Schottky gate structures, we observed an opposite trend, i.e., the V_{th} shift towards the negative gate voltage due to increasing x . From the numerical simulations of C-V curves using Poisson's equation supported by the analytical calculations of V_{th} , we showed that V_{th} shift in the examined MIS structures is due to a marked decrease in the positive Q_f with rising x . Finally, we examined the obtained dependencies of Q_f vs. x in terms of the different hypotheses proposed in the literature to explain the origin of the positive Q_f .

In our studies, we used AlGa_N/GaN MIS structures, as shown schematically in Fig. 1, which consist of 22 nm thick (d_i) SiO₂ and SiNx passivation layers and 25 nm thick (d_B) modulation doped Al_xGa_{1-x}N barrier layers ($x = 0.15, 0.26, 0.40$). We applied plasma-enhanced chemical vapor deposition (PECVD) and electron cyclotron resonance chemical vapor deposition (ECR CVD) techniques for the fabrication of SiO₂ and SiN layers, respectively. All heterojunction samples were cleaned with a HF solution before the insulator deposition in order to mitigate native oxides at the air-exposed AlGa_N surfaces. Ohmic contacts were ring-shaped Ti/Al/Ti/Au multilayers, and gate contacts were either Al/Au or Ni/Au circles with diameters from 200 to 500 μ m. An ohmic annealing was carried out at 830 °C for 2 min in N₂.

Figure 2 shows the experimental C-V curves of the SiO₂/Al_xGa_{1-x}N/GaN and SiN/Al_xGa_{1-x}N/GaN structures

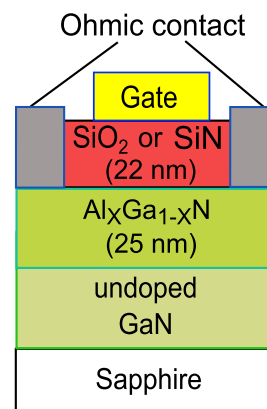


FIG. 1. Scheme of the cross-section of examined AlGa_N/GaN MIS structures.

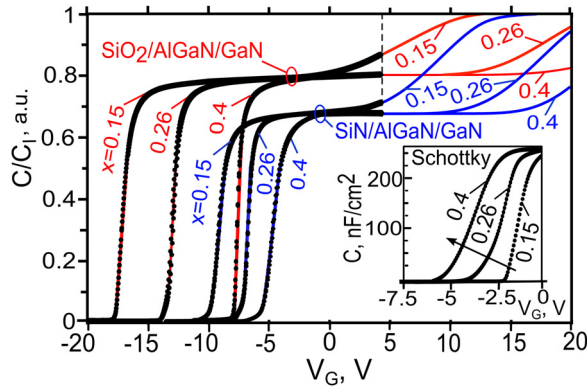


FIG. 2. Experimental (black points limited by the vertical dashed line) and theoretical (solid lines) C-V characteristics of the $\text{SiO}_2/\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ and $\text{SiN}/\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ structures. In the inset, for comparison, shown measured C-V curves of the Schottky gate structures. C_i is the insulator capacitance (for SiO_2 , $C_i = 130 \text{ nF/cm}^2$, and for SiN , $C_i = 240 \text{ nF/cm}^2$). The solid lines calculated assuming $D_{it}(E)$ from Figs. 3(b) and 3(c).

obtained at 1 MHz and at RT using an HP4192 impedance analyzer. The bias voltage was changed from -20 V to $+4 \text{ V}$ for the $\text{SiO}_2/\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ structures and from -15 V to $+4 \text{ V}$ for the $\text{SiN}/\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ structures. In the case of both types of structures, we observed a significant V_{th} shift in C-V curves towards the more positive gate voltage with increasing x . In particular, for $\text{SiO}_2/\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ structures, an increase of x from 0.15 to 0.4 caused the V_{th} shift from -17 to -7.5 V and for $\text{SiN}/\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ structures from -9.5 to -5 V . Due to such a large shift, we could observe typical of MISH structures two-step C-V curves^{2,3,18} only in the case of $x = 0.15$. In addition, for comparison, in the inset of Fig. 2, we also present the results of C-V

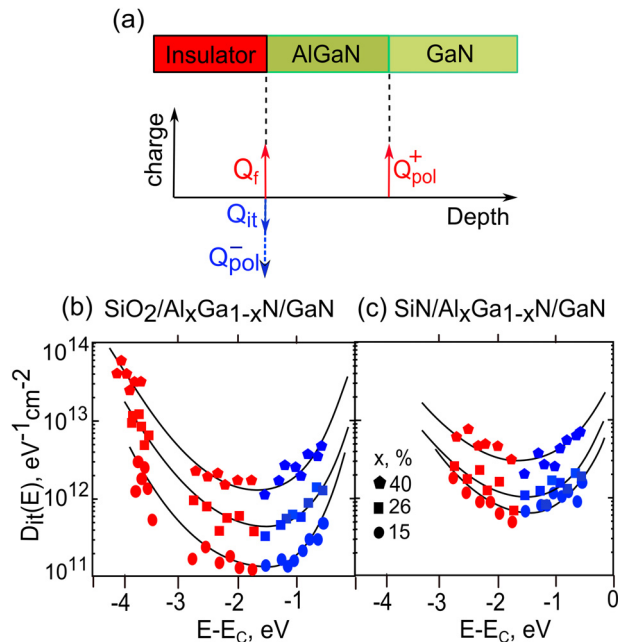


FIG. 3. Scheme of the charge distribution in AlGaIn/GaN MIS structures (a), $D_{it}(E)$ at $\text{SiO}_2/\text{Al}_x\text{Ga}_{1-x}\text{N}$ interfaces (Ref. 15) (b) and $D_{it}(E)$ at $\text{SiN}/\text{Al}_x\text{Ga}_{1-x}\text{N}$ interfaces (c) used in the calculations of C-V curves. In the case of $\text{SiO}_2/\text{Al}_x\text{Ga}_{1-x}\text{N}$, Q_{it}^f (in C/m^2) is 2.1×10^{-4} , 6.3×10^{-4} , and 2×10^{-3} for $x = 0.15$, 0.26, and 0.4, respectively, and in the case of $\text{SiN}/\text{Al}_x\text{Ga}_{1-x}\text{N}$, Q_{it}^f (in C/m^2) is 1.1×10^{-3} , 1.9×10^{-3} , and 4.8×10^{-3} for $x = 0.15$, 0.26, and 0.4, respectively.

TABLE I. The values of Q_{pol}^+ and Q_{pol}^- used in calculations.

x	Q_{pol}^+ (C/m^2)	Q_{pol}^- (C/m^2)
0.15	0.015	-0.035
0.26	0.022	-0.044
0.4	0.035	-0.06

measurements for the Schottky gate structures. One can note that V_{th} in this case exhibits an opposite behavior, i.e., the shift towards the more negative gate voltage with increasing x .

In order to explain the above results, we carried out the theoretical calculations of C-V curves based on solving a Poisson's equation. The details of calculations can be found in Refs. 15 and 19. In the calculations, we took into account the following charges, shown schematically in Fig. 3(a): (i) net positive polarization charge (Q_{pol}^+) at the AlGaIn/GaN interface originating from the spontaneous polarization of AlGaIn and GaN as well as piezoelectric polarization of AlGaIn , (ii) interface state charge (Q_{it}) at the insulator/ AlGaIn interface related to the interface state density distribution ($D_{it}(E)$) and (iii) net fixed charge (Q_{fnet}) at the insulator/ AlGaIn interface, which includes Q_f and the negative polarization charge, Q_{pol}^- , originating from the spontaneous and piezoelectric polarization of AlGaIn . We did not take into account the bulk charge in SiO_2 because we showed recently¹⁵ from the photo-assisted C-V measurements that this charge can be negligible in the case of the investigated structures. In addition, based on our recent studies of the surface photovoltage effect,²⁰ we also neglected the bulk charge in SiN . It was possible because in the case of the SiN/GaN structure, we observed a very fast recovery time of the surface photovoltage after turn-off of the ultraviolet light, which indicated the lack of the charge trapping effects in the SiN bulk. The values of Q_{pol}^+ and Q_{pol}^- for different x were taken from Ref. 21 and summarized in Table I. Furthermore, in the calculations, we assumed that the metal barrier height (ϕ_b) for Al/SiO_2 and Al/SiN was 3.7 eV (Ref. 22) and 2 eV (Ref. 22), respectively. The other parameters used in the calculations, i.e., the conduction band (CB) off-sets for the insulator/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$ junction [$\Delta E_{C1}(x)$] and $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ [$\Delta E_{C2}(x)$] are listed in Tables II and III, respectively. The value of $\Delta E_{C1}(x)$ was estimated from the following relationship:²² $\Delta E_{C1}(x) = \Delta E_{C3} - \Delta E_{C2}(x)$, where ΔE_{C3} is the conduction-band off-set for the insulator/ GaN junction [ΔE_{C3} for SiO_2/GaN is 3.6 eV (Ref. 22) and for SiN/GaN is 1.2 eV (Ref. 22)].

The solutions were obtained with: (i) Neumann type boundary conditions at the insulator/ AlGaIn and $\text{AlGaIn}/$

TABLE II. Conduction band off-sets, $\Delta E_{C1}(x)$, at insulator/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$ interfaces.

Interface	$\Delta E_{C1}(x)$ (eV)
$\text{SiO}_2/\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}$	3.28
$\text{SiO}_2/\text{Al}_{0.26}\text{Ga}_{0.74}\text{N}$	3.11
$\text{SiO}_2/\text{Al}_{0.4}\text{Ga}_{0.6}\text{N}$	2.88
$\text{SiN}/\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}$	0.87
$\text{SiN}/\text{Al}_{0.26}\text{Ga}_{0.74}\text{N}$	0.72
$\text{SiN}/\text{Al}_{0.4}\text{Ga}_{0.6}\text{N}$	0.48

TABLE III. Conduction band off-sets, $\Delta E_{C2}(x)$, at $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interfaces.²¹

Interface	$\Delta E_{C2}(x)$ (eV)
$\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}/\text{GaN}$	0.32
$\text{Al}_{0.26}\text{Ga}_{0.74}\text{N}/\text{GaN}$	0.48
$\text{Al}_{0.4}\text{Ga}_{0.6}\text{N}/\text{GaN}$	0.72

GaN interfaces and (ii) Dirichlet type boundary conditions at the contacts. In particular, the boundary conditions at the insulator/AlGaIn interface are expressed as

$$\epsilon_0 \epsilon_B E_B - \epsilon_0 \epsilon_I E_I = Q_{it} + Q_{fnet}, \quad (1)$$

where E_B and E_I is the electric field intensity in AlGaIn and insulator, respectively, ϵ_B and ϵ_I is the relative AlGaIn and insulator permittivity, respectively ($\epsilon_B = 10.3$, for SiO_2 $\epsilon_I = 3.9$ and for SiN $\epsilon_I = 7$); Q_{it} can be expressed as follows:

$$Q_{it} = q \int_{E_V}^{E_{CNL}} D_{it}(E)(1 - f_{it})dE - q \int_{E_{CNL}}^{E_C} D_{it}(E)f_{it}dE, \quad (2)$$

where E_V and E_C are the top of the valence band (VB) and bottom of the conduction band (CB), respectively, E_{CNL} is the charge neutrality level, and f_{it} is the Fermi-Dirac function. In the calculations, we used $D_{it}(E)$ at $\text{SiO}_2/\text{Al}_x\text{Ga}_{1-x}\text{N}$ interfaces from our recent paper¹⁵ [shown in Fig. 3(b)]. In the case of $\text{SiN}/\text{Al}_x\text{Ga}_{1-x}\text{N}$ interfaces, $D_{it}(E)$ was determined from the photo-assisted C-V method^{3,15} and then summarized in Fig. 3(c). The details of the measurements can be found in Refs. 2, 3, and 15. As a light source, we used a xenon lamp and a set of band-pass filters (the passing photon energy: $1.26 \text{ eV} < h\nu < 3 \text{ eV}$). During the calculations of C-V curves, we assumed that Q_{it} cannot follow the fast ac voltage signal but can follow the slow gate voltage sweep (high-frequency measurement).

While the shift of V_{th} in the Schottky structures towards the negative gate voltage with increasing x (Fig. 2) is obviously due to an increase of the positive Q_{pol}^+ , the shift of V_{th} in MIS AlGaIn/GaN structures towards the positive voltage with x can be due to either an increase of the negative Q_{pol}^- and Q_{it} or/and a decrease of the positive Q_f . Therefore, to determine which of these factors can be responsible for the V_{th} shift, first we calculated the C-V curves for the $\text{SiO}_2/\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ and $\text{SiN}/\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ structures with $x = 0.15$ and 0.40 , assuming, for both x , the same Q_f value equal to $|Q_{pol}^-|$ for $x = 0.15$ (see Table I). Such an approach allowed to examine, if the solely variations of Q_{pol}^- and Q_{it} vs. x can have the stronger impact on V_{th} than increasing of the positive polarization charge Q_{pol}^+ and thus, in consequence, if they can induce the V_{th} shift towards the positive gate voltage. The results of the V_{th} calculations are summarized in Fig. 4(a). It is evident from this figure that the C-V curves are shifted with increasing x towards the more negative voltage. This means that in order to induce the V_{th} shift towards the positive bias (Fig. 2), the significant reduction of the positive Q_f vs. x is necessary. From the fitting of the experimental C-V curves by the theoretical ones (Fig. 2), we estimated exactly the values of Q_f at $\text{SiO}_2/\text{Al}_x\text{Ga}_{1-x}\text{N}$ and

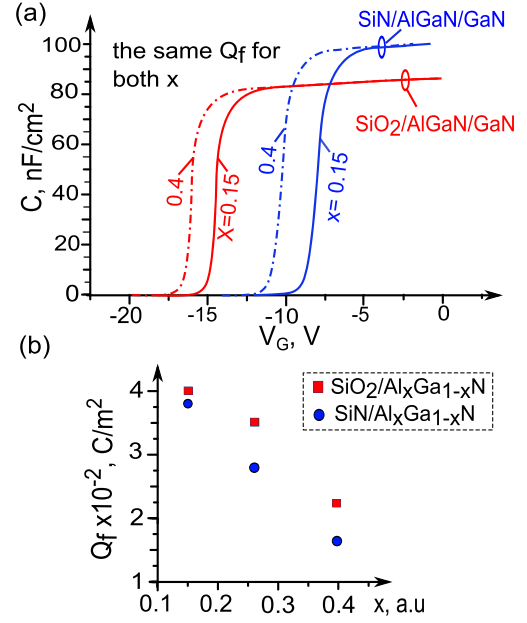


FIG. 4. C-V characteristics of the $\text{SiO}_2/\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ and $\text{SiN}/\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ structures with $x = 0.15$ and 0.4 calculated assuming, for both x , the same Q_f value equal to $|Q_{pol}^-|$ for $x = 0.15$ (see Table I) and $d_B = d_I = 30 \text{ nm}$ (a); dependencies of Q_f vs. x , determined from fitting of the experimental C-V curves (see Fig. 2) (b).

$\text{SiN}/\text{Al}_x\text{Ga}_{1-x}\text{N}$ interfaces and summarized them in Fig. 4(b) and Table IV. We found that in the case of $\text{SiO}_2/\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$, an increase of x from 0.15 to 0.4 caused reducing Q_f from 0.04 to 0.022 C/m^2 and in the case of $\text{SiN}/\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$, from 0.038 to 0.016 C/m^2 . In addition, it should be noted that the theoretical calculations of C-V curves for the examined structures with $x = 0.26$ and 0.4 indicate that the second step at these curves should occur much beyond the measured gate voltage range (see Fig. 2). This confirms that the lack of observation of the second step of C-V curves for these structures is due to the large shift of C-V curves towards the positive gate voltage with x but not due to high $D_{it}(E)$. Moreover, as one can note from Fig. 2, the second step of C-V curves in the case of the structures with $x = 0.15$, was well reproduced using $D_{it}(E)$ from Figs. 3(b) and 3(c). This gives an additional independent support for $D_{it}(E)$ determined from the photo-assisted C-V method.

It should be stressed that the values of Q_f obtained from the simulations of C-V curves can be confirmed through the analytical calculations of V_{th} using the model proposed by Tapajna and Kuzmik²³ Namely, within this model, V_{th} can be expressed as follows:

TABLE IV. The values of Q_f determined (a) from C-V fitting (Fig. 2) and (b) from Eq. (4).

Interface	(a) $Q_f \times 10^{-2} (\text{C/m}^2)$	(b) $Q_f \times 10^{-2} (\text{C/m}^2)$
$\text{SiO}_2/\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}$	4.05	4.08
$\text{SiO}_2/\text{Al}_{0.26}\text{Ga}_{0.74}\text{N}$	3.52	3.56
$\text{SiO}_2/\text{Al}_{0.4}\text{Ga}_{0.6}\text{N}$	2.17	2.20
$\text{SiN}/\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}$	3.77	3.79
$\text{SiN}/\text{Al}_{0.26}\text{Ga}_{0.74}\text{N}$	2.76	2.81
$\text{SiN}/\text{Al}_{0.4}\text{Ga}_{0.6}\text{N}$	1.65	1.62

$$V_{th} = \frac{\phi_b}{q} - \frac{\Delta E_C}{q} - \frac{\phi_f}{q} - \frac{d_I}{\epsilon_I} (Q_{pol}^-) - \frac{d_I \epsilon_B + d_B \epsilon_I}{\epsilon_I \epsilon_B} (Q_{pol}^+) - \frac{d_I}{\epsilon_I} (Q_f + Q_{it}^{fr} + Q_I^{bulk}), \quad (3)$$

where ϕ_f is the Fermi potential in the GaN bulk (~ 0.2 eV), Q_I^{bulk} is the insulator bulk charge, and Q_{it}^{fr} is the charge corresponding to the “frozen” interface states³ between E_{CNL} and 0.8 eV from E_C ($Q_{it}^{fr} \approx -q \int_{E_{CNL}}^{0.8\text{eV}} D_{it}(E) dE$). The values of Q_{it}^{fr} are given in the caption of Fig. 3.

For our structures, Q_I^{bulk} can be neglected (as mentioned before); therefore, from Eq. (3), we can estimate Q_f as follows:

$$Q_f \approx \frac{\epsilon_I}{d_I} \left(\frac{\phi_b}{q} - \frac{\Delta E_C}{q} - \frac{\phi_f}{q} - V_{th} \right) - (Q_{pol}^-) - \frac{d_I \epsilon_B + d_B \epsilon_I}{d_I \epsilon_B} (Q_{pol}^+) - Q_{it}^{fr}. \quad (4)$$

After substituting into Eq. (4) the values from Tables I to III as well as the values of Q_{it}^{fr} (see the caption of Fig. 3) and V_{th} , we calculated Q_f , as shown in Table IV. It is clear from this table that we obtained a good agreement with the values determined from the fitting of C-V curves.

In order to understand the obtained dependencies of Q_f vs. x [Fig. 4(b)], we examined the different hypotheses proposed in the literature to explain the origin of the positive Q_f at the insulator/III-N interfaces, which are schematically illustrated in Fig. 5. At first, we considered the hypothesis developed by Ganguly *et al.*,¹² denoted here as hypothesis A. According to this hypothesis, Q_f is related to the Al-O bonds at the interface. On the other hand, it should be noted that it was observed experimentally that the density of Al-O bonds at the AlGaN surface increases with x due to the enhancement of the chemical affinity of aluminum to oxygen.²⁴ Therefore, from hypothesis A it follows that one should expect an increase of Q_f vs. x , which is in contradiction with our observation. Another hypothesis, introduced by Hayashi *et al.*²⁵ and Tapajna and Kuzmik²³ (hypothesis B) suggests that Q_f is linked to the ionized donor-like surface defects formed during the growth on the III-N heterostructure. Furthermore, it was shown by Gordon *et al.*²⁶ that the concentration of donor-like surface defects increases with

increasing x ; thus within hypothesis B, one should also observe, contrary to our results, an enlargement of Q_f vs. x . The next hypothesis, developed by Bakroot *et al.*¹⁷ (hypothesis C), assigned Q_f to the gate insulator border trap. Concerning this hypothesis, one should consider two cases: (i) when the border trap responsible for Q_f is located close to the insulator/AlGaN interface inside the disordered interface region, and (ii) when the border trap is located far from the interface. In the case (i), the border trap density (D_{BT}) should increase with x like $D_{it}(E)$ at the SiO₂/AlGaN and SiN/AlGaN interfaces [Figs. 3(b) and 3(c)]. On the contrary, in the case (ii), D_{BT} should depend weakly on x . Therefore, according to hypothesis C, Q_f can increase or can be rather independent on x , against to our finding. The last hypothesis proposed by Esposto *et al.*¹³ (hypothesis D), postulates that Q_f originates from the energy states between CB bottom of the AlGaN and insulator layer. Only this hypothesis is able to explain the observed variations of Q_f vs. x . Namely, if we assume the continuous distribution of the above states, then it is evident that Q_f can be approximately expressed by the following relationship (see Fig. 5):

$$Q_f \approx q D_{CB} \Delta E_{C1}(x), \quad (5)$$

where D_{CB} is the average density of states between the edge of CB of an insulator and AlGaN.

Because $\Delta E_{C1}(x)$ at the SiO₂/Al_xGa_{1-x}N and SiN/Al_xGa_{1-x}N interfaces decreases with increasing x (see Table II), thus from Eq. (5), it follows that Q_f should also decrease with x . Moreover, the independent support for the hypothesis D comes from our recent studies based on the photo-assisted C-V measurements.¹⁵ Namely, we showed that the states between CB of SiO₂ and AlGaN can be fully ionized and thus they can behave like the fixed charge.

Finally, it is worth to highlight the important finding of our work that Q_f can be precisely controlled by the barrier composition [as in Fig. 4(b)]. In particular, Figs. 2 and 4(b) suggest that by using an appropriate high x , in the case of SiO₂/AlGaN/GaN and SiN/AlGaN/GaN structures, one can obtain a reduced Q_f to the negligible value and, as a result, shifting V_{th} to the region of the positive gate voltage, which ensures normally off operation.²

In conclusion, we found that the positive fixed charge Q_f at the insulator/Al_xGa_{1-x}N interfaces exhibits a significant decrease with increasing x , which results in the V_{th} shift towards the positive gate voltage. We examined this result with respect to the various hypotheses developed in the literature to explain the origin of the positive Q_f at insulator/III-N interfaces. We showed that the hypothesis proposing that Q_f originates from the energy states between the CB bottom of an insulator and AlGaN is the most suitable for the explanation of our data. We believe that the revealed dependence of Q_f on x can be useful for the tuning V_{th} in AlGaN/GaN MISHEMTs.

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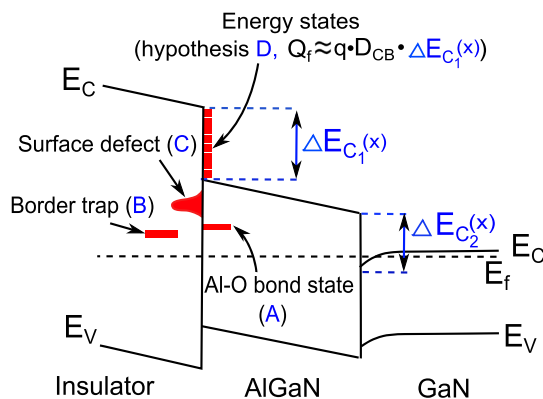


FIG. 5. Schematic illustration of the hypotheses^{12,13,17,23,25} (A–D) proposed to explain the origin of the positive Q_f at the insulator/III-N interfaces.

to the calculations. The work was realized within the SAFEMOST project, Visegrad Group (V4)—Japan Joint Research Program on Advanced Materials (in Poland, the NCRD Project, No. 14/990/PNN16/0072).

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