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Insulator-semiconductor interface fixed charges in AlGaN/GaN metal-insulator-semiconductor devices with Al_2O_3 or AlTiO gate dielectrics

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We have investigated insulator-semiconductor interface fixed charges in AlGaN/GaN metal-insulator-semiconductor (MIS) devices with Al_2O_3 or AlTiO (an alloy of Al_2O_3 and TiO_2) gate dielectrics obtained by atomic layer deposition on AlGaN. Analyzing insulator-thickness dependences of threshold voltages for the MIS devices, we evaluated positive interface fixed charges, whose density at the AlTiO/AlGaN interface is significantly lower than that at the Al_2O_3/AlGaN interface. This and a higher dielectric constant of AlTiO lead to rather shallower threshold voltages for the AlTiO gate dielectric than for Al_2O_3. The lower interface fixed charge density also leads to the fact that the two-dimensional electron concentration is a decreasing function of the insulator thickness for AlTiO, whereas being an increasing function for Al_2O_3. Moreover, we discuss the relationship between the interface fixed charges and interface states. From the conductance method, it is shown that the interface state densities are very similar at the Al_2O_3/AlGaN and AlTiO/AlGaN interfaces. Therefore, we consider that the lower AlTiO/AlGaN interface fixed charge density is not owing to electrons trapped at deep interface states compensating the positive fixed charges and can be attributed to a lower density of oxygen-related interface donors. *Published by AIP Publishing.* https://doi.org/10.1063/1.5017668

I. INTRODUCTION

GaN-based heterojunction field-effect transistors (HFETs)[1] are important devices owing to their high current drive capability and high breakdown voltages. However, there are several disadvantages of GaN-based HFETs; self-heating effects,[2–4] current collapse phenomena,[5,6] and also gate leakage currents are limiting factors for the practical use of these devices. For the suppression of gate leakage currents and the current collapse phenomena in GaN-based devices, it can be effective to employ metal-insulator-semiconductor (MIS) structures, which are also significant to normally off operations,[7] even though GaN-based MIS devices sometimes exhibit unstable characteristics.[8–12] As a gate dielectric of GaN-based MIS devices, high-dielectric-constant (high-k) insulators, such as Al_2O_3,[13] HfO_2,[14,15] TaON,[16] AlN,[17–21] BN,[22,23] and AlTiO,[24] have been investigated. In GaN-based MIS device processing, when an insulator is deposited on a negatively polarized III-N semiconductor surface, such as Ga-face (Al)GaN, positive insulator-semiconductor interface fixed charges tend to be generated and to cancel the negative polarization charges.[25–32] However, the existence of the insulator-semiconductor interface fixed charges is not a necessity.[29,30] Since the interface fixed charges have significant impacts on threshold voltages V_{th}, we expect that V_{th} can be controlled by "interface charge engineering,"[29] i.e., by controlling the interface fixed charges. In particular, if the positive interface fixed charge density is sufficiently suppressed, a normally off operation can be expected.[33,34] However, despite many reports on the interface fixed charges, their sufficient control is a remaining issue. Moreover, their origin is not fully elucidated even though they are attributed to positively ionized oxygen donors in some cases. Therefore, further investigations on insulator-semiconductor interface fixed charges for GaN-based MIS devices are very necessary and important towards V_{th} control and normally off operations.

In this work, we investigated insulator-semiconductor interface fixed charges in AlGaN/GaN MIS devices with Al_2O_3 or AlTiO (an alloy of Al_2O_3 and TiO_2[35–37]) gate dielectrics, which are deposited on an AlGaN/GaN heterostructure by atomic layer deposition (ALD). AlTiO has, depending on its composition, intermediate physical properties between Al_2O_3 ($k \sim 9$ and $E_g \sim 7$ eV) and TiO_2 ($k \sim 60$ and $E_g \sim 3$ eV),[37] being useful to balance the trade-off between k and energy gap E_g. Previously, we fabricated AlTiO/AlGaN/GaN MIS devices with excellent characteristics, indicating that AlTiO can be an important candidate for a gate dielectric of GaN-based MIS devices.[24] The present work involves a comparative study on insulator-semiconductor interface fixed charges in Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices. By analyzing linear insulator-thickness dependences of V_{th}, we evaluated insulator-semiconductor interface fixed charges. As a result, we find that the fixed charge density at the AlTiO/AlGaN interface is significantly lower than that at the Al_2O_3/AlGaN interface. In addition, we also discuss the relationship between the interface fixed charges and interface states. It is suggested that the lower AlTiO/AlGaN interface fixed charge density is not owing to electrons trapped at deep interface states.

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II. DEVICE FABRICATION

Using an $Al_{0.27}Ga_{0.73}N$(30 nm)/GaN(3000 nm) heterostructure grown by metal-organic vapor phase epitaxy on sapphire(0001), we fabricated AlGaN/GaN MIS devices with Al_2O_3 or AlTiO gate dielectrics. The device fabrication was started with Ti/Al/Ti/Au Ohmic electrode formation. After surface treatments using organic solvents, oxygen plasma ashing, and an ammonium-based solution, insulator films of Al_2O_3 or AlTiO as gate dielectrics with several thicknesses $d_{ins} = 6$–29 nm were deposited on the AlGaN surface by ALD. The Al_2O_3 films ($k \sim 9$ and $E_g \sim 7$ eV) were obtained by using trimethylaluminum (TMA) and H_2O as precursors, and the Al_xTi_yO films (x:y = 0.73:0.27, $k \sim 13$–14, and $E_g \sim 6$ eV) were by using TMA, tetrakis-dimethylamino titanium (TDMAT), and H_2O. After post-deposition annealing in H_2-mixed Ar at 350 °C, Ni/Au gate electrode formation completed the device fabrication. As a result, we obtained Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices, whose cross sections are schematically shown in Fig. 1(a), with 70 μm × 70 μm gate electrodes surrounded by the Ohmic electrodes as shown by top-view optical images in Fig. 1(b).

III. INSULATOR-SEMICONDUCTOR INTERFACE FIXED CHARGES

In order to investigate insulator-semiconductor interface fixed charges, we examined threshold voltages V_{th} of the Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices, by measuring capacitance-voltage (C–V) characteristics between the gate and the grounded Ohmic electrodes. Since GaN-based MIS devices sometimes exhibit unstable V_{th} depending on the sweeping range of the gate voltage V_G,[8–12] we checked V_{th} stability; starting from $V_{G0} \geq 0$, C–V characteristics were measured under $V_G = V_{G0} \rightarrow -15$ V with a sweep rate of 0.36 V/s. Figure 2 shows an example of the

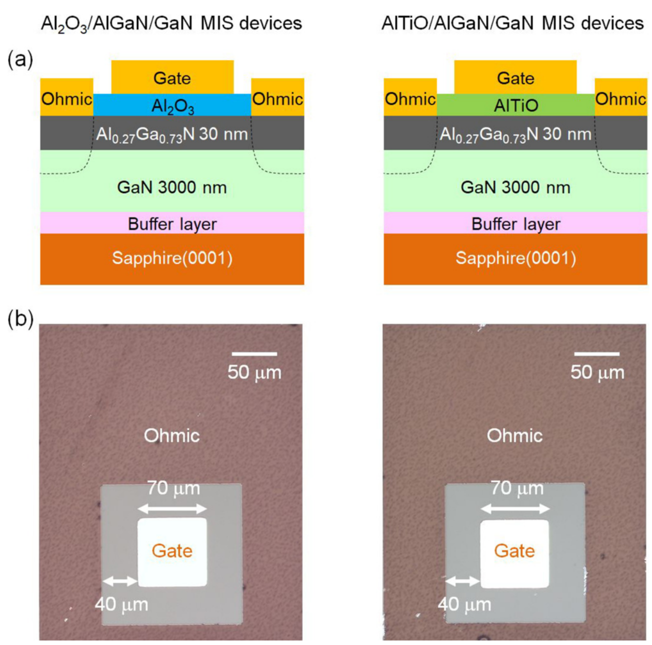

FIG. 1. (a) Schematic cross sections and (b) top-view optical images of the fabricated Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices.

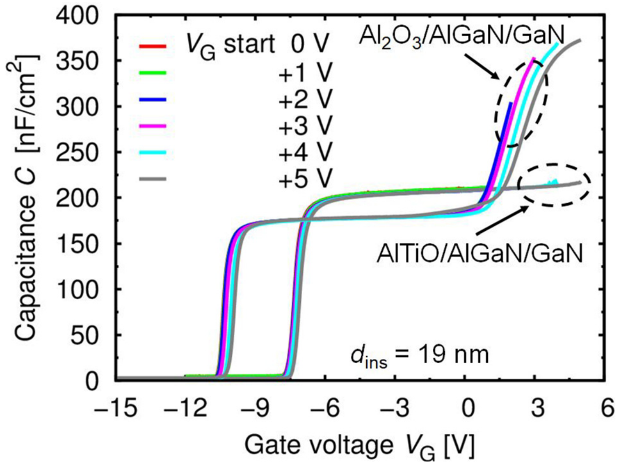

FIG. 2. Checking V_{th} stability of the Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices with $d_{ins} = 19$ nm: C–V characteristics measured at 1 MHz under $V_G = V_{G0} \rightarrow -15$ V with a sweep rate of 0.36 V/s, where $V_{G0} = 0$, 1, 2, 3, 4, and 5 V.

measurement results for $d_{ins} = 19$ nm, at 1 MHz frequency with $V_{G0} = 0$, 1, 2, 3, 4, and 5 V. Although we find rather stable V_{th}, weak V_{th} shifts take place after positive bias applications, probably owing to charging effects of trapped electrons. Thus, to determine V_{th}, we employ $V_{G0} = 0$ V to avoid the charging effects. Figure 3(a) shows C–V characteristics of the MIS devices with $d_{ins} = 6$–29 nm, measured at 1 MHz under $V_G = 0 \rightarrow -15$ V with a sweep rate of 0.36 V/s. As shown in Fig. 3(b), the sheet concentration of the two-dimensional electron gas (2DEG) under the gate, n_s, can be obtained by integrating C as a function of V_G, from which we can determine V_{th}.

Figure 4 shows the band diagram of AlGaN/GaN MIS devices, considering the interface fixed charges. From this, we obtain

$$\frac{\Delta\sigma_{ins} - qn_s}{k_{ins}\varepsilon_0} d_{ins} + \frac{\Delta\sigma_{AlGaN} - qn_s}{k_{AlGaN}\varepsilon_0} d_{AlGaN} = -V_G + \psi/q + E_F/q \quad (1)$$

using the elementary charge $q > 0$, the vacuum permittivity ε_0, the insulator-semiconductor interface fixed charge density σ_{ins}, the polarization charge densities σ_{GaN} and σ_{AlGaN}, the dielectric constants k_{ins} and k_{AlGaN}, the thicknesses d_{ins} and d_{AlGaN}, the 2DEG Fermi energy E_F, and $\psi = \phi - \varphi - \Delta E_C$ defined in Fig. 4, where $\Delta\sigma_{ins} = \sigma_{ins} - \sigma_{GaN}$ and $\Delta\sigma_{AlGaN} = \sigma_{AlGaN} - \sigma_{GaN}$. For $V_G = V_{th}$ ($n_s = 0$ and $E_F = 0$), we find

$$V_{th} = -\frac{\Delta\sigma_{ins}}{k_{ins}\varepsilon_0} d_{ins} - \frac{\Delta\sigma_{AlGaN}}{k_{AlGaN}\varepsilon_0} d_{AlGaN} + \psi/q \quad (2)$$

giving a linear d_{ins}-dependence of V_{th} with a slope of $-\Delta\sigma_{ins}/(k_{ins}\varepsilon_0)$. The 2DEG concentration n_s under the gate is approximately given by

$$qn_s \simeq C_0(V_G - V_{th}) \quad (3)$$

as experimentally confirmed in Fig. 3(b), where

$$\frac{1}{C_0} = \frac{d_{ins}}{k_{ins}\varepsilon_0} + \frac{d_{AlGaN}}{k_{AlGaN}\varepsilon_0}. \quad (4)$$

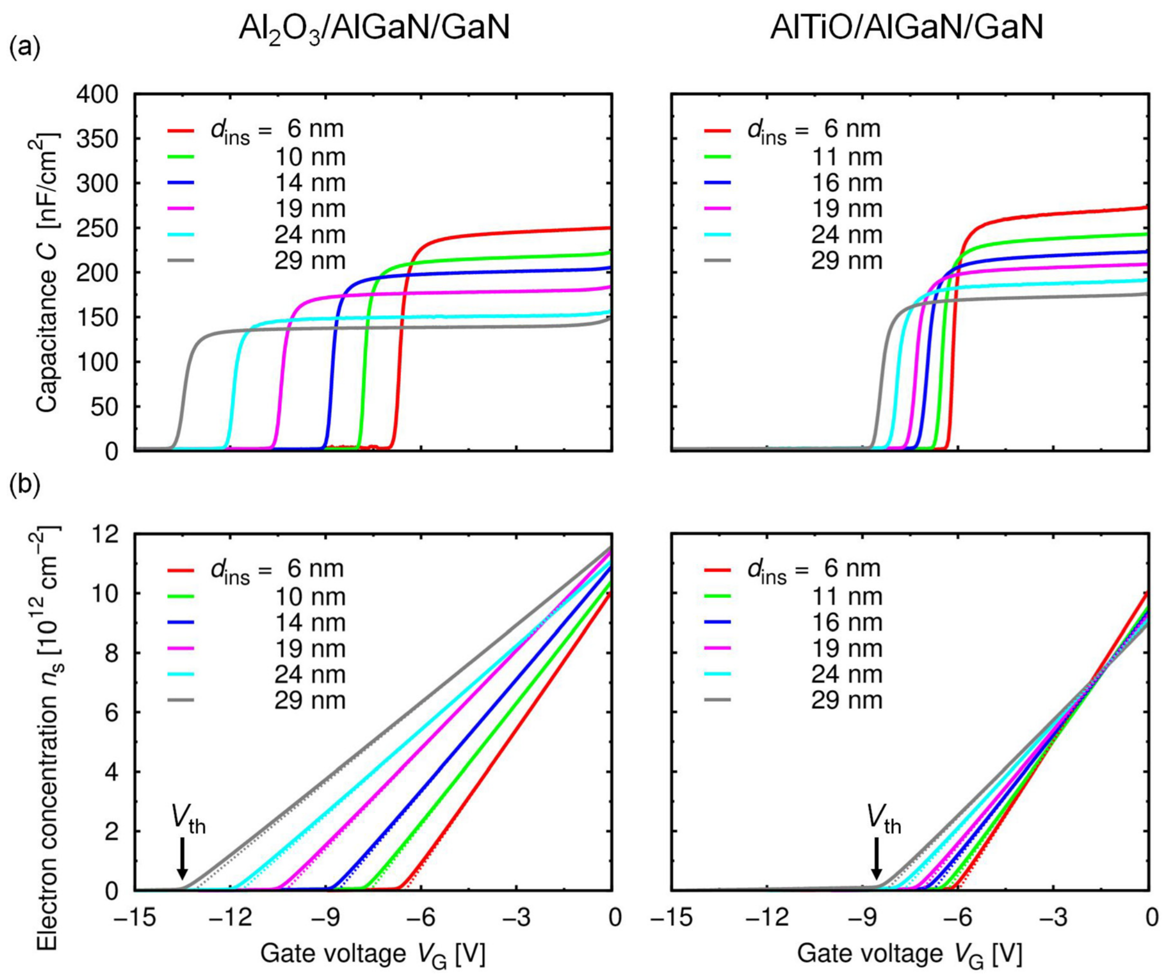

FIG. 3. (a) C–V characteristics of the Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices with $d_{ins} = 6$–29 nm, measured at 1 MHz under $V_G = 0 \rightarrow -15$ V with a sweep rate of 0.36 V/s. (b) The 2DEG sheet concentration n_s obtained by integrating C as functions of the gate voltage V_G, from which we can determine V_{th}.

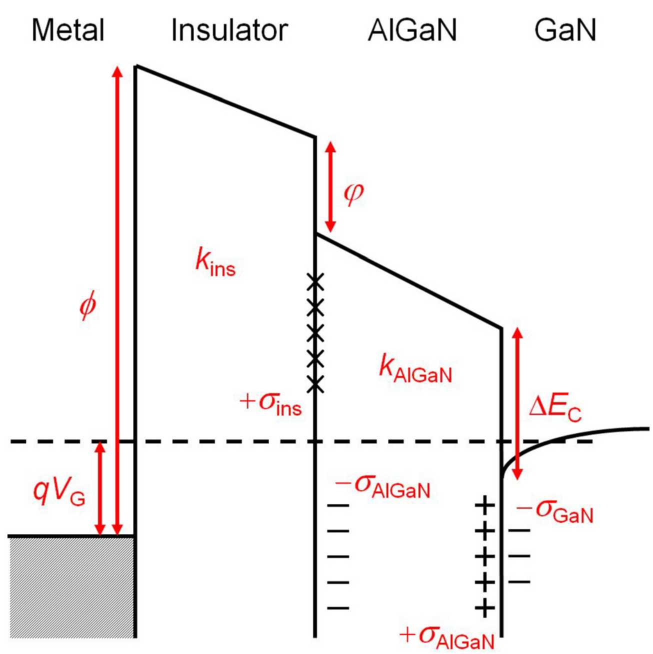

FIG. 4. The band diagram of AlGaN/GaN MIS devices, considering the interface fixed charges.

For $V_G = 0$, $n_s = n_{s0}$ is given by

$$qn_{s0} \simeq -C_0 V_{th} = \frac{\Delta\sigma_{ins} d_{ins}/(k_{ins}\varepsilon_0) + \Delta\sigma_{AlGaN} d_{AlGaN}/(k_{AlGaN}\varepsilon_0) - \psi/q}{d_{ins}/(k_{ins}\varepsilon_0) + d_{AlGaN}/(k_{AlGaN}\varepsilon_0)} \tag{5}$$

which is a nonlinear function of d_{ins}.

According to Eq. (4), $1/C_0$ is a linear function of d_{ins}. Experimentally, C_0 is estimated by C at $V_G = 0$ V as plotted in Fig. 5(a), where we can confirm the linear relation. From the slopes, we obtain dielectric constants $k_{ins} = 9.4$ and 13.4 for Al_2O_3 and AlTiO, respectively, being consistent with separated experimental results using metal-insulator-metal structures (not shown). From the intercept, we obtain $k_{AlGaN} = 9.5$ (using $d_{AlGaN} = 30$ nm). Figure 5(b) shows the experimentally determined V_{th} as functions of d_{ins}. We find linear dependences obeying Eq. (2), indicating that the interface fixed charges dominate V_{th} and also rather shallower V_{th} for AlTiO than for Al_2O_3. By fitting using Eq. (2), we obtain $\Delta\sigma_{ins}/q = 1.5 \times 10^{13}$ cm^{-2} and 7.3×10^{12} cm^{-2} at the Al_2O_3/AlGaN and AlTiO/AlGaN interfaces, respectively. The latter gives a significantly lower σ_{ins} than the former, which may be attributed to a lower-density of oxygen donors[25,31,32] at

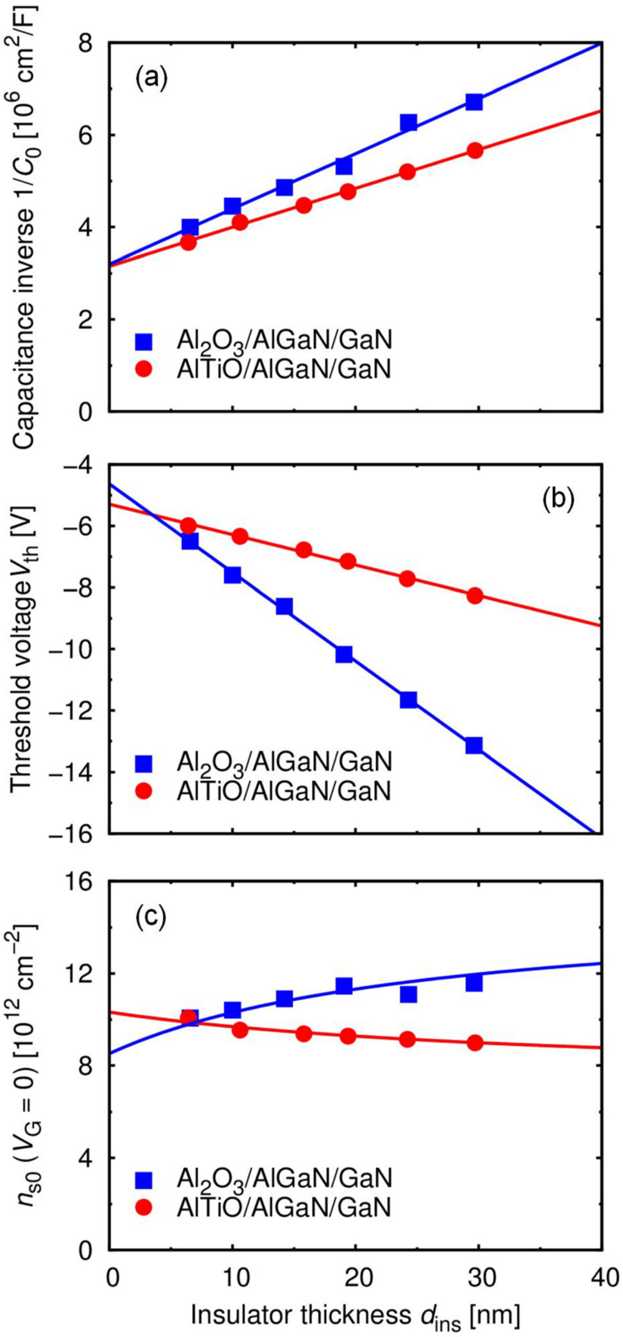

FIG. 5. (a) $1/C_0$, (b) V_{th}, and (c) n_{s0} at $V_G = 0$ of the Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices, as functions d_{ins} with fitting curves.

the AlTiO/AlGaN interface. This lower σ_{ins} and the higher k_{ins} of AlTiO lead to rather shallower V_{th}. Figure 5(c) shows the experimentally obtained n_{s0} as functions of d_{ins}, whose non-linear dependences are fitted by Eq. (5). We find that n_{s0} is a decreasing function of d_{ins} for AlTiO, whereas being an increasing function for Al_2O_3. From Eq. (5), we obtain

$$\frac{\partial n_{s0}}{\partial d_{ins}} = \frac{C_0}{k_{ins}\varepsilon_0}(\Delta\sigma_{ins}/q - n_{s0}) \qquad (6)$$

which implies that $\Delta\sigma_{ins}/q > n_{s0}$ leads to increasing n_{s0} with d_{ins}, while $\Delta\sigma_{ins}/q < n_{s0}$ leads to decreasing n_{s0}. Thus, for Al_2O_3 and AlTiO, n_{s0} is an increasing and a decreasing function of d_{ins}, respectively. It should be noted that, in the limit of a large d_{ins}, n_{s0} in Eq. (5) approaches to $\Delta\sigma_{ins}/q$, indicating that a normally off operation can be expected for sufficiently suppressed interface fixed charges, satisfying $\Delta\sigma_{ins} < 0$, i.e., $\sigma_{ins} < \sigma_{GaN}$. However, in the both cases, we observe $\Delta\sigma_{ins} > 0$, i.e., $\sigma_{ins} > \sigma_{GaN}$.

Even though $\Delta\sigma_{ins}$ is obtained experimentally, in order to evaluate σ_{ins}, it is necessary to assume σ_{GaN}. Hereafter, we assume $\sigma_{GaN}/q = 2.1 \times 10^{13}\,\mathrm{cm}^{-2}$ obtained by a theoretical calculation.[38] This leads to $\sigma_{ins}/q = 3.6 \times 10^{13}\,\mathrm{cm}^{-2}$ and $2.8 \times 10^{13}\,\mathrm{cm}^{-2}$ at the Al_2O_3/AlGaN and AlTiO/AlGaN interfaces, respectively. In addition, these values should be compared with σ_{AlGaN}/q. Although $\Delta\sigma_{AlGaN}/q = 1.5 \times 10^{13}\,\mathrm{cm}^{-2}$ for $Al_{0.27}Ga_{0.73}N$/GaN is obtained theoretically,[39] several experiments show lower $\Delta\sigma_{AlGaN}$, about 85% of the theoretical one.[40–42] Thus, we assume $\Delta\sigma_{AlGaN}/q = 1.3 \times 10^{13}\,\mathrm{cm}^{-2}$, i.e., $\sigma_{AlGaN}/q = 3.4 \times 10^{13}\,\mathrm{cm}^{-2}$. Based on the assumptions, we summarize σ_{ins} compared with σ_{AlGaN} in Fig. 6, where the dotted line corresponds to neutral insulator-semiconductor interfaces, i.e., $\sigma_{ins} + (-\sigma_{AlGaN}) = 0$. We obtain that the Al_2O_3/AlGaN interface is nearly neutral,[25] while the AlTiO/AlGaN interface is rather negatively charged owing to the lower σ_{ins}. By fitting V_{th} as functions of d_{ins} with Eq. (2), we also obtain $\psi = 2.0$ and 1.3 eV for the Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices, respectively. From these, we obtain band diagrams of the AlGaN/GaN MIS devices by Poisson-Schrödinger calculation[43] as shown in Fig. 7, where we can confirm that the AlTiO/AlGaN interface is negatively charged. The directions of the electric fields in Al_2O_3 and AlTiO at $V_G = 0$ V are opposite, leading to the fact that n_{s0} is a decreasing function of d_{ins} for AlTiO, whereas being an increasing function for Al_2O_3.

IV. RELATION WITH INSULATOR-SEMICONDUCTOR INTERFACE STATES

It should be noted that electrons trapped at deep interface states with very long time constants can act as (quasi) negative interface fixed charges.[30] Therefore, the interface fixed charge measurements might be influenced by electrons at deep interface states compensating the positive fixed

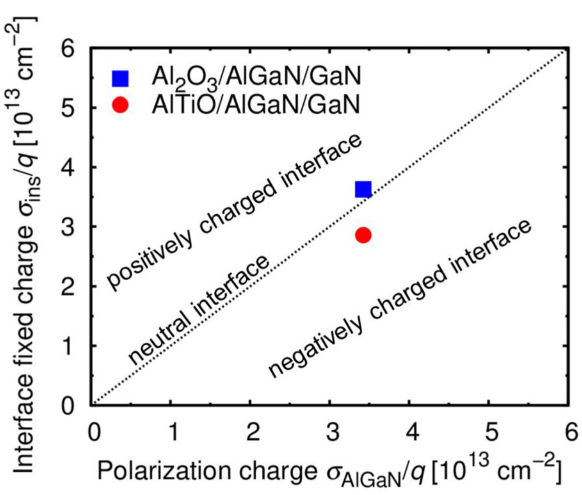

FIG. 6. A comparison between the insulator-semiconductor interface fixed charge density σ_{ins} and AlGaN polarization charge density σ_{AlGaN}.

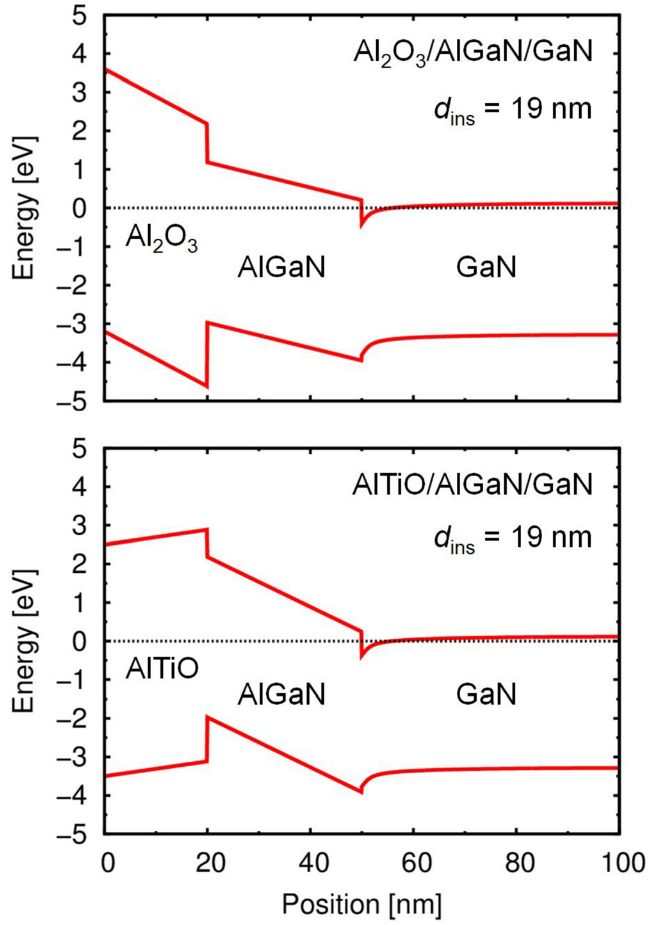

FIG. 7. Band diagrams of the Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices at $V_G = 0$ V, obtained by 1D Poisson-Schrödinger calculation.

charges. In particular, there is a possibility that the lower AlTiO/AlGaN interface fixed charge density is owing to electrons trapped at deep interface states. In order to consider this possibility, we examined the interface states at Al_2O_3/AlGaN and AlTiO/AlGaN by frequency dependent C–V measurements. Figure 8 shows examples of the measurement results, C–V characteristics at 100 Hz–1 MHz for the Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices with $d_{ins} = 14$–19 nm. In any cases, no frequency dispersion is observed for negative bias voltages, showing that the V_{th} determination is not affected by the measurement frequency. On the other hand, for positive bias voltages, frequency dispersions are observed, suggesting insulator-semiconductor interface states.

The conductance method[44] was applied to the frequency dependent C–V characteristics to evaluate the interface state density.[30,45–51] Assuming the equivalent circuit shown in the insets of Fig. 9, which consists of an interface state capacitance C_i, an interface state conductance G_i, and an AlGaN capacitance C_{AlGaN} in parallel, with an insulator capacitance C_{ins} connected in series, we obtained the frequency dependence of G_i for the Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices. Figure 9 shows examples of obtained G_i/ω as functions of frequency f, where $\omega = 2\pi f$, exhibiting single-peaked behavior. As shown by the curves in Fig. 9, the single-peaked behavior is well fitted by[52]

$$\frac{G_i}{\omega} = \frac{q^2 D_i \ln(1+\omega^2\tau^2)}{2\omega\tau}, \tag{7}$$

where D_i is the interface state density and τ is the trapping time constant, giving the peak frequency $f_p = 1/(\pi\tau)$ and the peak value of $G_i/\omega \simeq 0.4q^2 D_i$. The observed peaks are summarized in Fig. 10(a), where we find very similar behavior

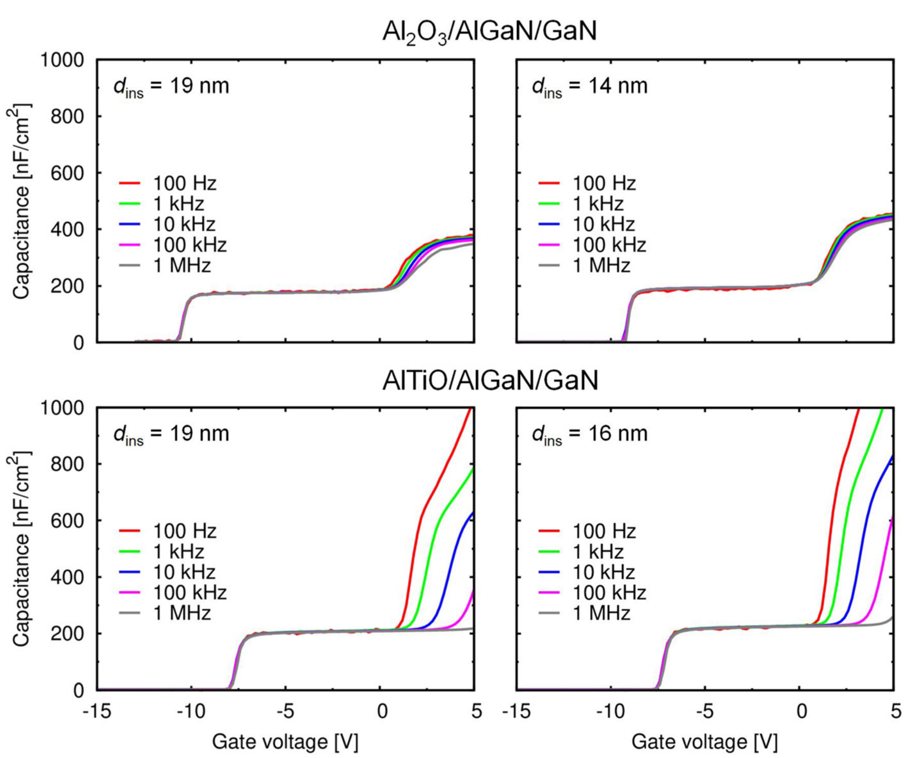

FIG. 8. C–V characteristics of the Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices with $d_{ins} = 14$–19 nm, measured at 100 Hz–1 MHz.

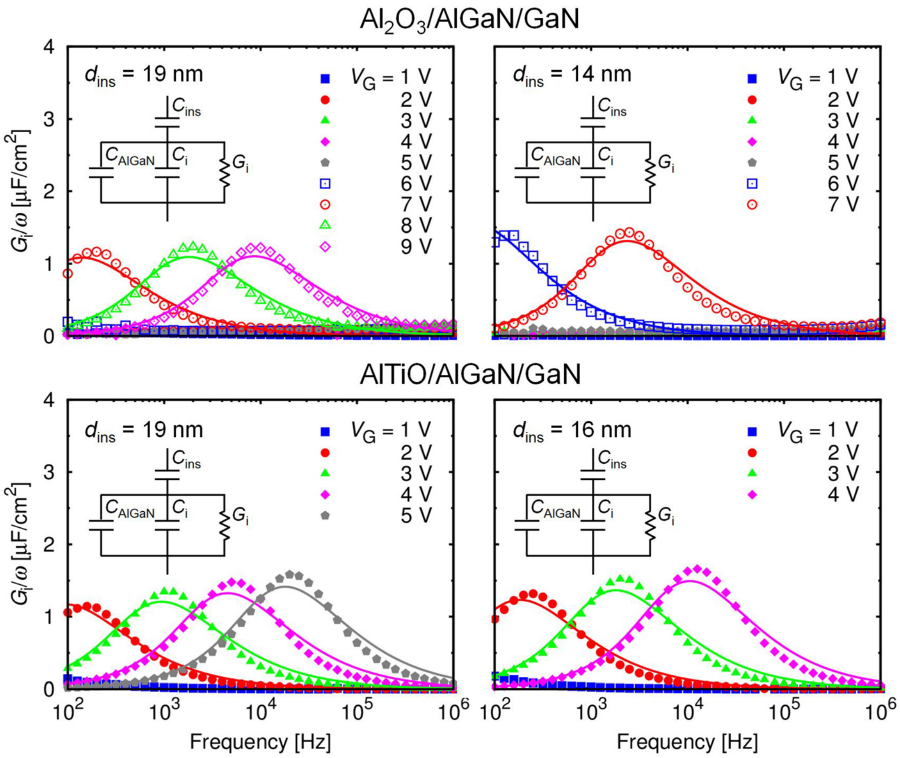

FIG. 9. G_i/ω as functions of frequency with fitting curves for the Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices. Insets: The small-signal equivalent circuit.

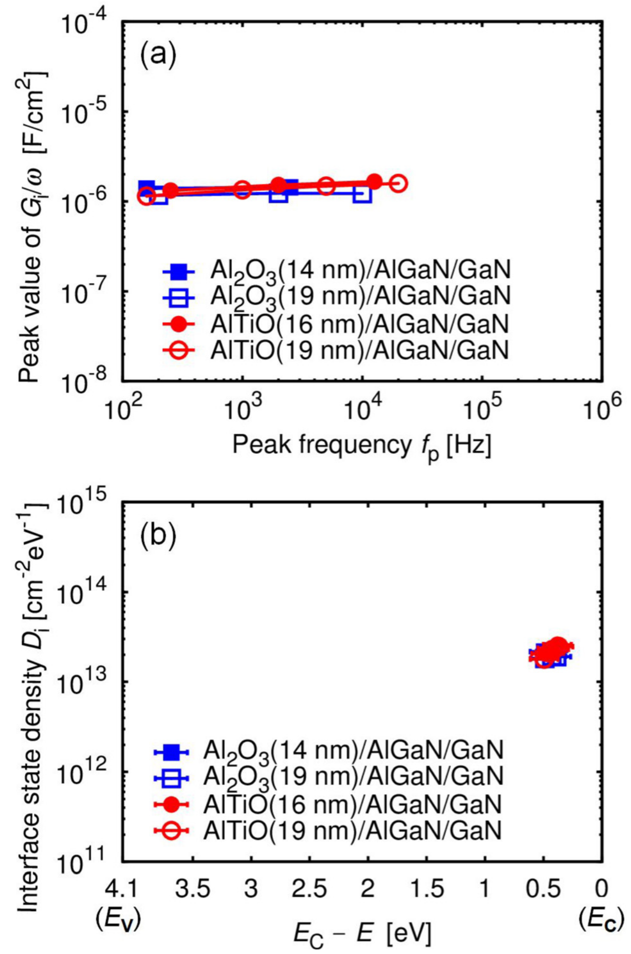

FIG. 10. (a) The peak value of G_i/ω as functions of peak frequency f_p and (b) the interface state density D_i as functions of the energy $(E_C - E)$, for the Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices.

for Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN and also for different d_{ins}, suggesting that the behavior is dominated by interface states with very similar densities at Al_2O_3/AlGaN and AlTiO/AlGaN. From the peaks, we can obtain the relationship between D_i and τ. Moreover, τ for an interface state at the energy E is given by $\tau = \tau_0 \exp[(E_C - E)/k_B T]$ using the Boltzmann constant k_B, temperature T, and the conduction band bottom energy E_C, where τ_0 is a time constant determined by the capture cross section of the trap. Thus, using τ_0, we can estimate the relationship between D_i and $(E_C - E)$. Even though τ_0 is ambiguous, assuming a wide range of $\tau_0 = 1$–100 ps, we show D_i as functions of $(E_C - E)$ in Fig. 10(b), where the error bars correspond to the wide range of τ_0 values. This indicates a very similar shallow interface state density $D_i \sim 2 \times 10^{13}\,\mathrm{cm^{-2}eV^{-1}}$ of Al_2O_3/AlGaN and AlTiO/AlGaN and suggests that deep interface state densities are also similar, even though the interface fixed charge density σ_{ins} is rather lower at AlTiO/AlGaN. Thus, we should conclude that there is no correlation between the interface fixed charges and the interface states in our case, as reported in Ref. 32. This suggests that the lower σ_{ins} at AlTiO/AlGaN is not owing to electrons trapped at deep interface states, compensating the positive fixed charges. Since interface states generally have a U-shaped density of states, from the shallow interface state density above, we can expect a deep interface state density of $\lesssim 10^{13}\,\mathrm{cm^{-2}eV^{-1}}$ or less. On the other hand, the difference between σ_{ins}/q at Al_2O_3/AlGaN and that at AlTiO/AlGaN is $\sim 0.8 \times 10^{13}\,\mathrm{cm^{-2}}$. Thus, it is not plausible that the difference is due to trapped electrons at the deep interface states. Although the material origin of the lower σ_{ins} at AlTiO/AlGaN is not clear, it is possible to tentatively assume a lower density of oxygen-related interface donors, where strong Ti-O bonding may suppress donor formation.

V. CONCLUSION

We have investigated insulator-semiconductor interface fixed charges in Al_2O_3/AlGaN/GaN and AlTiO/AlGaN/GaN MIS devices. The AlTiO/AlGaN interface gives significantly lower-density interface fixed charges and rather shallower threshold voltages. The lower interface fixed charge density also leads to the fact that the 2DEG concentration is a decreasing function of the AlTiO thickness, whereas being an increasing function of the Al_2O_3 thickness. Moreover, we discuss the relationship between the interface fixed charges and interface states. Since the interface state densities are very similar at Al_2O_3/AlGaN and AlTiO/AlGaN, it is suggested that the lower interface fixed charge density at AlTiO/AlGaN is not owing to electrons trapped at deep interface states, compensating the positive fixed charges. Thus, a lower density of oxygen-related donors at the AlTiO/AlGaN interface can be assumed, where strong Ti-O bonding may suppress donor formation. We consider that the results can provide a clue towards V_{th} control and normally off operations of GaN-based MIS devices.

ACKNOWLEDGMENTS

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