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Direct measurement of donor-like interface state density and energy distribution at insulator/AlGaN interface in metal/Al2O3/AlGaN/GaN by photocapacitance method

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Direct measurement of donor-like interface state density and energy distribution at insulator/AlGaN interface in metal/Al₂O₃/AlGaN/GaN by photocapacitance method

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We determined the energy distribution of donor-like interface state density \( D_{it} (E) \) at the Al₂O₃/AlGaN interface in a metal/Al₂O₃/AlGaN/GaN heterostructure (MISH) capacitor. In this order, we developed a point-by-point graphical method based on the measurement and simulations of the MISH photocapacitance versus ultraviolet light intensity. We found a tail-like shaped \( D_{it} (E) \) strongly decreasing from the value of \( 5 \times 10^{15} \text{ cm}^{-2} \) in the energy range between 0.12 eV and 0.45 eV from the AlGaN valence band edge.

The impact of electronic states at the insulator/AlGaN interface on AlGaN/GaN based devices, e.g., metal/insulator/semiconductor heterostructure field effect transistors (MISHFETs) has been well established. The interface states semiconductor heterostructure field effect transistors (MISH) have been developed recently, which were considered, namely a discrete distribution \( D_{it} \) in the AlGaN band gap. It should be stressed that the interface state density distribution at insulator/AlGaN interface in metal/Al₂O₃/AlGaN/GaN heterostructure (MISH) capacitors because of two interfaces and extremely long time constants for charge emission from the deep states at room temperature (RT). Recently, from the capacitance-voltage (C–V) hysteresis and photo-assisted C–V the interface states \( D_{it} (E) \) distributed around the AlGaN midgap and acceptor-like states near the conduction band edge \( (E_C) \) were reported. However, the energy distribution of the donor interface state density at the AlGaN surface is completely unknown.

In this letter, we determined directly the donor-like interface state density distribution \( D_{it} (E) \) at the Al₂O₃/AlGaN interface in a metal/Al₂O₃/AlGaN/GaN MISH capacitor in the energy range between 0.12 eV and 0.45 eV from the valence band edge \( (E_V) \). In this order, we modified our method based on the measurement and simulations of the photocapacitance \( (C_L) \) versus excitation ultraviolet (UV) light intensity \( (Φ) \), which was recently developed by Matys et al. for the determination of the donor-like interface states in Al₂O₃/GaN MIS. Here, from a graphical approach, we obtained \( D_{it} (E) \) in a point-by-point manner.

The investigated Al₂O₃ (20 nm)/Al₀.₂₅Ga₀.₇₅N (30 nm)/GaN structure was intentionally undoped (electron concentration in AlGaN of \( 5 \times 10^{15} \text{ cm}^{-3} \)). The Ni/Al (20/50 nm) gate was circular, and Ti/Al/Ti/Al ohmic contact was ring shaped. The Al₂O₃ passivation layer was grown by atomic layer deposition at 350 °C. The scheme of the studied MISH capacitor structure and technological details are described in Ref. 13. The photocapacitance for the gate bias \( V_G \) from −4.0 to −2 V was measured at 1 MHz at RT. In addition, the surface photovoltage (SPV) at the Al₂O₃/AlGaN interface, i.e., the change in the contact potential difference upon illumination, was registered using the Besocke Kelvin probe. As a light source, a xenon lamp and a band-pass filter \( (λ = 300 \text{ nm}) \) were applied. The exemplary \( C_L \) transients after switch on and off the light, for \( V_G = −3 \text{ V} \), are shown in Fig. 1(a). One can note that the steady-state \( C_L \) response for higher \( Φ \) was achieved after longer time. In the measurement of \( C_L (Φ) \) dependencies to assure the steady-state \( C_L \), for all \( Φ \) we assumed a period of about 60 min, as for the largest \( Φ \). After UV off a very slow decrease of the \( C_L \) signal was observed. This transient can be attributed to the long restoring of the potential barrier at the Al₂O₃/AlGaN interface, which was reduced under UV illumination. This effect is probably determined by the change in the interface charge due to slow capturing electrons emitted thermionically from 2DEG. The time dependence of barrier recovery was proven from the SPV transient measured for nonbiased structure (Fig. 1(b)). After 50 min of UV off (with different intensity) the C–V measurements were performed, first in the \( V_G \) range from −3 to −14 V, and then from −14 to 6 V. From Fig. 1(c), it results that the obtained C–V curves exhibit the parallel shift (larger after higher \( Φ \)) towards the negative voltage. This shift is due to a widening of the energy range of the interface states, which changes their total charge \( Q_B \) upon UV illumination and behave as a fixed charge after UV switch off. The dependence of C–V voltage shift (\( ΔV \)) versus \( Φ \) is shown in Fig. 1(d). We found...
that this dependence is expressed by the relationship \( \Delta V \sim \Phi^{0.042} \). The full structure reset was realized by applying a positive bias \( V_G = 6 \) V necessary to attract electrons from the AlGaN/GaN interface to Al2O3/AlGaN interface, where they are captured by the interface states. It should be mentioned that the measured photo and dark leakage current was negligibly small (less than 20 nA/cm²) for the photocapacitance experiment.

Our method for the determination of the donor \( D_{id}(E) \) is based on the following model of non-equilibrium effects in an Al2O3/AlGaNoGaMISH. The structure illuminated with photon energy above AlGaN band gap is biased with the negative \( V_G \) for which the corresponding total structure capacitance \( C_{\text{dark}} \) in the dark is equal to \( C_{\text{dark}}^{-1} = C_{\text{AlGaN}}^{-1} + C_{\text{Al2O3}}^{-1} \), where \( C_{\text{AlGaN}} \) and \( C_{\text{Al2O3}} \) is the capacitance of the AlGaN and Al2O3, respectively. On the other hand, \( V_G \) should be negative enough to quench the interface recombination at Al2O3/AlGaN, similarly to the case of Al2O3/GaN interface, as we proved in our previous work.14 Under excitation the MISH total photocapacitance \( (C_L) \) changes with respect to the dark value \( (C_{\text{dark}}) \) due to \( C_{\text{AlGaN}} \) variations. This is because excess electrons and holes are separated in the electrical field in AlGaN (scheme in Fig. 2). The holes are attracted towards the Al2O3/AlGaN interface, whereas electrons are both repelled by the negative \( V_G \) and attracted by the positive fixed charge at the AlGaN/GaN interface. Furthermore, due to the positive valence band offset16 (VBO) of Al2O3 with respect to AlGaN the flow of photoholes through dielectric film is impossible. The holes are captured by the donor-like interface states, which become positively ionized. On the contrary, the deep acceptor-like states, if exist, are not ionized due to lack of electrons at the interface but become neutralized due to hole capturing. Upon increasing \( \Phi \) and rising number of excess holes, the hole quasi-Fermi level at the interface, \( E_{Fh} \), scans the widening range of interface states distributed in the AlGaN band gap. In contrast, the electron quasi-Fermi level, \( E_{Fe} \), is almost constant at the interface.

For the calculation of the Al2O3/AlGaNoGaMISH photocapacitance, we used one-dimensional drift-diffusion model.15 We assumed that the generation rate decreases exponentially versus the distance from the interface with different absorption coefficients in AlGaN and GaN layers. We took into account all main bulk recombination channels, i.e., radiative band-to-band recombination, non-radiative Shockley-Read-Hall (SRH) recombination, transitions through deep acceptor levels in GaN (related to so-called yellow photoluminescence, PL) and also interface recombination through the interface states distributed at the Al2O3/AlGaN interface, in terms of the SRH statistics as described in Ref. 14. The AlGaN and GaN bulk parameters for these calculations were taken from Ref. 1 and parameters used in the relationships describing yellow PL in GaN from Ref. 18. We assumed different donor \( D_{id}(E) \) and acceptor-like \( D_{ia}(E) \) interface state density distributions in the whole AlGaN bandgap at the Al2O3/AlGaN interface and neglected the states at AlGaN/GaN one. In addition, the net interface fixed charge \( Q_{\text{net}} \) at the Al2O3/AlGaN interface (polarization charge and ionized defects) and the fixed polarization charge \( Q_p \) were taken into account.

The sheet density of the total charge \( Q_{\text{fit}} \) at the Al2O3/AlGaN interface is described by the following formula:

\[
Q_{\text{fit}} = Q_{\text{id}} + Q_{\text{ia}} = \int_{E_V}^{E_C} D_{id}(E)(1 - f_i) q \, dE - \int_{E_V}^{E_C} D_{ia}(E)f_i q \, dE, \tag{1}
\]

where \( Q_{\text{id}} \) is the donor-like state charge and \( Q_{\text{ia}} \) is the acceptor-like state charge; \( f_i \) is the occupation function taken from Ref. 14.

At the Al2O3/AlGaNoGaMISH interfaces, we used the Neumann boundary conditions. Namely, at the Al2O3/AlGaN interface

\[
\begin{align*}
\frac{d\Phi}{dx} & = 0, \\
\frac{d\rho}{dx} & = 0, \quad \text{at} \quad x = 0, \\
\frac{d\Phi}{dx} & = 0, \quad \text{at} \quad x = d, \\
\frac{d\rho}{dx} & = 0, \quad \text{at} \quad x = d, \\
\Phi & = 0, \quad \text{at} \quad x = 0, \\
\rho & = 0, \quad \text{at} \quad x = d.
\end{align*}
\]

FIG. 1. Relative \( C_L \) transients of AlGaN MISH at RT for \( \Phi_1 \) (curve 1) > \( \Phi_2 \) (curve 2) (a), SPV transient (b), C–V curves measured in the dark after illumination with increasing intensity \( \Phi \) (c), and voltage shift of C–V curves versus \( \Phi \) (d).

FIG. 2. Illuminated and negatively biased AlGaN/GaN MISH, (1, 4) electron-hole generation in AlGaN and GaN, respectively, (2, 5) band-to-band recombination, (3, 6) non-radiative bulk SRH recombination, (7) radiative point defect transitions, and (8) hole capturing by interface states.
\[ \varepsilon_{Al} \varepsilon_0 E_{Al} - \varepsilon_{Si} \varepsilon_0 E_{Si} = Q_{it} + Q_{net}, \]  

(2)

where \( \varepsilon_{Al} \) is the AlGaN and Al2O3 dielectric constant, respectively, \( \varepsilon_0 \) is the vacuum permittivity, \( E_{Al} \) is the electric field intensity in AlGaN and insulator, respectively.

Boundary conditions at the contacts are the Dirichlet type, i.e., at the gate (\( x = 0 \)) \( V = V_G - \phi_s/q + \phi_b/q \), where \( V_G \) is the gate voltage, \( \phi_s \) is the surface barrier height (for Ni/Al2O3, \( \phi_s = 3.5 \) eV), and \( \phi_b \) is the built-in potential (in eV), respectively, and \( V = 0 \) at the Ohmic contact. The boundary conditions for the continuity equations are given in terms of the interface recombination rate. In the \( C_L \) calculation, like in Ref. 14, we assumed that the interface state charge cannot follow the fast AC voltage signal (h-f measurement). The model equations were solved self-consistently using a finite element method with the very good convergence (relative error at the level of \( 10^{-6} \)) to obtain the in-depth distribution of electric potential and carrier densities in MISH.

In order to determine \( D_{id}(E) \) at the Al2O3/AlGaN interface, the analysis of Al2O3/AlGaN/GaN MISH photocapacitance \( C_L \) and main Al2O3/AlGaN interface electronic parameters versus \( \Phi \), i.e., \( E_{FP} \), excess hole concentration \( p_s \), and \( Q_{id}(E) \) was performed. In the analysis, we neglected \( D_{id}(E) \) because they do not influence the \( C_L \) response as it will be proven in the experimental result discussion. The results of calculations for the structure biased with \( V_G = -3 \) V and various \( D_{id}(E) \) distributions (flat and exponential) in the AlGaN band gap are shown in Figs. 3(a)–3(e).

From Fig. 3(a), it is evident that a given \( C_L \) value (in terms of \( \Delta C = C_L - C_{dark} \)) can be reproduced by means of different \( D_{id}(E) \) distributions (point A in Fig. 3(a)). It results from the fact that for all relevant \( D_{id}(E) \), the total number of holes captured by donor-like states for a given \( \Phi \) (corresponding to point A), and thus, the actual interface \( E_{FP} \) position in the AlGaN band gap must be the same. This is supported by the calculations, which give the same value of \( p_s \) and \( Q_{id}(E) \) at point A for the different \( D_{id}(E) \) as shown in Figs. 3(b) and 3(c). All these prove that for an exemplary \( C_L(\Phi) \) curve calculated for an exponential \( D_{id}(E) \) function, we can find a set of the equivalent flat \( D_{id}(E) \) distributions as well as corresponding \( Q_{id}(E) \), \( p_s \), and, thus, \( E_{FP} \). Therefore, the average local value of \( D_{id}(E) \) can be found from the relationship:

\[ D_{id}(E) = \frac{|Q_{id}^{\Phi,C} - Q_{id}^{\Phi,B}|}{E_{FP}^C - E_{FP}^B}, \]  

(3)

where \( Q_{id}^{\Phi,C} \) and \( E_{FP}^C \) are the values of interface donor charge and hole quasi-Fermi level corresponding to points B and C, respectively. On the basis of the above approach, we reproduced very well in point-by-point manner the assumed exponential curve \( D_{id}(E) \) (dots on the reproduced curve 1 in Fig. 3(d)). From Fig. 3(c), it results that the \( Q_{id}(\Phi) \) curves exhibit different slopes depending on the \( D_{id}(E) \) shape, i.e., the slope is larger for stronger \( D_{id}(E) \) increasing towards \( E_F \). In particular, \( Q_{id} \sim \Phi^{0.015} \) for all flat state density distributions. We also proved that the determined \( D_{id}(E) \) does not depend on both the net interface fixed charge \( Q_{net} \), and excess carrier lifetime \( \tau \). In this order, we analyzed \( Q_{id}(E_{FP}) \) dependencies (shown in Fig. 3(e)), which were obtained using the above method for curve 1 in Fig. 3(a), assuming different \( Q_{net} \). The calculation was performed for the positive \( Q_{net} \) taken from the literature. From Fig. 3(e), it results that \( Q_{net} \) causes a parallel shift of \( Q_{id}(E_{FP}) \) curves with respect to an \( E_{FP} \) axis without changing their slope. For larger \( Q_{net} \), the interface charge \( Q_{id} \) was lower because of the reduced number of holes at the Al2O3/AlGaN interface due to their repelling by \( Q_{net} \). Thus, the actual \( D_{id}(E) \) value (from Eq. (2)) is the same for various \( Q_{net} \). Analogously \( \tau \) influences the determined \( Q_{id}(E_{FP}) \) as it was proven from the simulations carried out for different \( \tau = 10^{-7} \) and \( 10^{-9} \) s. This is due to the constant quantum efficiency of the bulk SRH recombination rate in the analyzed \( \Phi \) range because of the negligible interface recombination.

Subsequently, we analyzed the experimental \( C_L(\Phi) \) dependencies upon UV excitation in order to determine \( D_{id}(E) \) at the Al2O3/AlGaN interface. It should be noted that these dependencies were measured for different \( V_G \) to extend the energy range of scanned interface states by shifting \( E_F \). At first, we excluded the possible contribution of the \( D_{id}(E) \) to \( C_L(\Phi) \) dependencies from the comparison of the experimental and simulated curves, as summarized in Fig. 4. It is evident that the \( C_L(\Phi) \) curve 1 corresponding to \( D_{id}(E) \) (\( Q_{net} < 0 \)) is shifted toward lower \( \Phi \) values with respect to the ideal curve. In contrary, curve 3 corresponding to \( D_{id}(E) \) (\( Q_{net} > 0 \)) is shifted toward higher \( \Phi \), the same like the experimental \( C_L(\Phi) \) curves (points), which are shifted even more by several orders of magnitude. One can also note that the shift of experimental curves is much larger than the shift due to the positive \( Q_{net} \). On this basis, we concluded that mainly \( D_{id}(E) \) are responsible for the experimental \( C_L(\Phi) \) responses. Then, we generated a set of \( C_L(\Phi) \) curves corresponding to flat \( D_{id}(E) \)
distributions, which pass through all experimental points, as shown in Fig. 4, and calculated \( D_{\text{ad}}(E) \) from Eq. (2). Additionally, from the measured \( C_{\text{L}}(\Phi) \) curves the \( Q_{\text{ad}}(\Phi) \) dependencies for different \( Q_{\text{net}} \) were determined and summarized in the inset in Fig. 5. One can note that the experimental \( Q_{\text{ad}}(\Phi) \) (despite of \( Q_{\text{net}} \)) and \( \Delta V(\Phi) \) curves are the same functions on \( \Phi \). This correlation is an additional support of the donor character of the observed interface states. The obtained \( D_{\text{ad}}(E) \) distribution at the examined \( \text{Al}_2\text{O}_3/\text{AlGaN} \) interface is presented in Fig. 5. One can note that the exponential function corresponding to the continuous states in the AlGaN bandgap result from the interfacial disorder of bond lengths and angles.

It should be noted that the presented method for determining \( D_{\text{ad}}(E) \) requires high-k insulating layers with positive \( V_{\text{BO}} \) and negligible leakage currents. However, it can also be implemented for ultrathin dielectric layers after taking into account a photo-hole tunneling. The case for dielectrics with negative \( V_{\text{BO}} \) will be analysed in our future work.

In conclusion, we determined quantitatively in a point-by-point manner the donor-like interface state density distribution \( D_{\text{ad}}(E) \) at the \( \text{Al}_2\text{O}_3/\text{AlGaN} \) interface which was impossible to achieve by other methods. In the near \( E_V \) region, the shape of \( D_{\text{ad}}(E) \) resembles a tail extending into the valence band. It should be stressed that the obtained result is crucial to understand the main electronic properties of both \( \text{AlGaN/GaN MIS} \) structures and free AlGaN surfaces as well as interface state origin. The method reported here can be easily applied for heterostructures of various wide band gap semiconductors. We thank R. Ucka, M.Sc. Eng., for his help in experiment.

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