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Quantitative observation and discrimination of AlGaN- and GaN-related deep levels in AlGaN/GaN heterostructures using capacitance deep level optical spectroscopy

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Deep levels were observed using capacitance deep level optical spectroscopy (DLOS) in an AlGaN/GaN heterostructure equivalent to that of a heterojunction field effect transistor. Band gap states were assigned to either the AlGaN or GaN regions by comparing the DLOS spectra in accumulation and pinch-off modes, where the former reflects both AlGaN- and GaN-related defects, and the latter emphasizes defects residing in the GaN. A band gap state at $E_c-3.85$ eV was unambiguously identified with the AlGaN region, and deep levels at $E_c-2.64$ eV and $E_c-3.30$ eV were associated with the GaN layers. Both the AlGaN and GaN layers exhibited additional deep levels with large lattice relaxation. The influence of deep levels on the two-dimensional electron gas sheet charge was estimated using a lighted capacitance-voltage method. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2424670]

Power amplifiers based on AlGaN/GaN heterojunction field effect transistors (HFETs) are hampered by defects attributed to the AlGaN surface[1–3] and the GaN buffer[4–6] that exert detrimental influence upon device performance. Thus, quantitative observation of band gap states in AlGaN/GaN heterostructures provides an important metric for optimizing material growth and minimizing the impact of defects. Previous investigations pragmatically used HFETs themselves as a vehicle to study deep levels in AlGaN/GaN heterostructures, primarily focusing on the influence that pulsing of the gate-source bias or drain-source bias has on deep level activity and consequent degradation of pulsed versus dc I-V characteristics due to diminished two-dimensional electron gas (2DEG) sheet charge n_s. Beyond those deep levels made apparent with bias modulation, additional band gap states can exist that affect n_s and thereby device performance equally for both steady-state, pulsed, and rf operation and thus might not be observed using pulsing-based spectroscopy techniques such as drain current deep level transient spectroscopy[2,3] (I-DLTS) or photoionization induced current transient spectroscopy[4–6] (PICTS). Moreover, current-based techniques offer limited direct information regarding the location of defects within the heterostructure.

Here, we applied capacitance deep level optical spectroscopy[7] (C-DLOS) to probe deep levels in Schottky diodes formed from an AlGaN/GaN heterostructure equivalent to that of a HFET. C-DLOS provides an advantage over drain current spectroscopy because the depth sensitivity inherent to capacitance measurements can discern deep levels associated with the AlGaN region from those of the underlying GaN layers through choice of the diode bias V_G. With the heterostructure biased at $V_G=0$ V (accumulation), C-DLOS readily detects deep levels located within both the AlGaN and GaN regions. Further, the availability of 2DEG electrons for capture suppresses deep level photoemission at the heterointerface. Conversely, when performed at V_G less than the threshold voltage (V_{th}) such that the 2DEG is depleted (pinch-off), the heterostructure behaves as a bulk depletion region constituted mainly by GaN, and the photocapacitance of band gap states in the AlGaN region and heterointerface is strongly diminished compared to those in the GaN. It is notable that the role of any surface states at the unmetalized AlGaN surface is negligible since the semitransparent Schottky contact defines the region responsive to C-DLOS under these conditions. Thus, using C-DLOS it is possible both to observe and to distinguish among deep levels associated with the AlGaN region and those corresponding to the underlying GaN.

Optical excitation is necessary to probe the AlGaN cap in capacitance mode, whereas the applicability of traditional DLTS is limited to regions where the Fermi level (E_F) position can be modulated with bias, which excludes the AlGaN layer. In accumulation charge control of the 2DEG senses change in deep level occupancy. Deep levels given to electron photoemission increase n_s and are referenced to the conduction band minimum E_c. Likewise, a decrease in the photocapacitance indicates hole emission referenced to the valence band maximum E_v. In addition to photoemission, electron-hole pair creation also can increase n_s, so one must distinguish between these mechanisms. The Franz-Keldysh effect due to the bias and polarization-induced electric fields in the AlGaN generates an effective "redshift" of the optically sensed band gap energy in C-DLOS but is expected to have little influence on deep level photoemission.[8]

The AlGaN/GaN heterostructure was grown on a SiC substrate by metal-organic chemical vapor deposition

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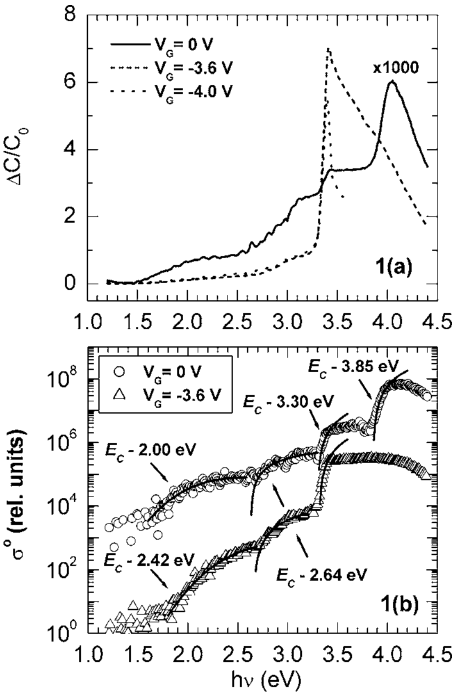

FIG. 1. (a) AlGaN/GaN SSPC spectra in accumulation (V_G=0 V) and pinch-off (V_G=−3.6,−4.0 V). Note the AlGaN band edge in accumulation and the GaN band edge at pinch-off. (b) DLOS spectra at V_G=0 and −3.6 V.

(MOCVD). Growth was initiated with an AlN nucleation layer followed by a 700 nm GaN:Fe semi-insulating buffer. Subsequently, 1700 nm of unintentionally doped (UID) GaN was deposited prior to the AlGaN (22 nm, 22% Al mole fraction) cap growth. Diodes were formed by evaporating an 8 nm Ni layer to provide a semitransparent Schottky contact and a Ti/Al/Ni/Au stack to form the Ohmic contact. An $n_s=6.2\times10^{12}$ cm^{-2} and a threshold voltage of −3.2 V were extracted from capacitance-voltage measurements. Hall data from a separate sample with the same structure grown on the same day yielded a mobility of 1900 cm^2/V s.

Measurements were conducted at 297 K at fixed V_G with monochromatic light ranging in energy from 1.20 to 4.40 eV with a 0.01 eV resolution using a Xe lamp source coupled with a high resolution monochromator. After equilibration in the dark, photocapacitance transients were recorded for steady-state photocapacitance (SSPC) and C-DLOS analysis. Inflection points in the SSPC spectrum approximately indicate deep level energy, and precise energies were obtained via C-DLOS by extracting emission rates from the transients and correcting for the photon flux to determine the spectral dependence of the optical cross section σ^o,[7] where it is assumed that either electron or hole emission dominates. Fitting σ^o to a theoretical model[7,9] determines the optical ionization energy E^o and, when relevant, the Franck-Condon energy $d_{\rm FC}$. Comprehensive discussion of DLOS is available elsewhere.[10]

Figure 1(a) displays the SSPC at V_G=0, −3.6, and −4 V. Unlike typical capacitance spectroscopy of uniformly doped bulk films, the increase in photocapacitance relative to the equilibrium value $\Delta C/C_0$ is not proportional to the areal deep level density D_t; consideration of D_t is given later. Considering the V_G=0 V spectrum, which can sense deep levels within both the AlGaN and GaN layers, several important features are apparent. The peak near $h\nu$=4.05 eV agrees with the expected AlGaN band edge for 22% mole fraction AlGaN and confirms sensitivity to the AlGaN cap. Positive inflection points in the spectrum near $h\nu$=1.5, 2.7, 3.3, and 3.9 eV indicate electron emission from deep levels, and the latter can be immediately ascribed to the AlGaN since this energy exceeds the GaN band gap. The origins of the other three defect levels were yet ambiguous, so additional measurements were performed at pinch-off to distinguish between GaN- and AlGaN-related band gap states.

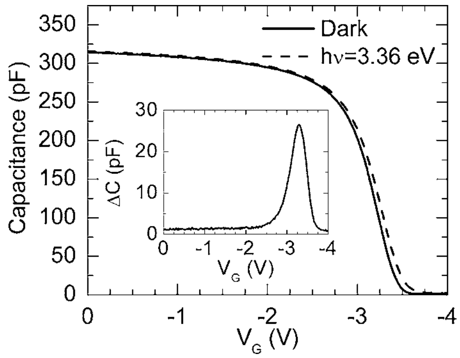

FIG. 2. Lighted capacitance-voltage scan for $h\nu$=3.36 eV denoting an increase in n_s. The inset shows the increase in capacitance ΔC with illumination as a function of V_G.

At V_G=−3.6 and −4 V the 2DEG is dissipated as seen from the dark *C*-*V* curve in Fig. 2, and the depletion depth extends into the GaN. In this case the relative thicknesses of the AlGaN (22 nm), UID-GaN (1700 nm), and GaN:Fe (700 nm) layers weight their contribution to the total photocapacitance. Thus, for $V_G<V_{\rm th}$, spectral features arising from the GaN region are strongly emphasized over those associated with the AlGaN. Indeed, appearance of the 3.44 eV GaN band edge peak confirms ascendancy of the photoresponse from the GaN layer. As expected, the distinctly AlGaN-related features, i.e., the 4.05 eV band edge peak and the 3.9 eV onset, quench. The lack of the AlGaN band edge in the SSPC spectra at pinch-off implies that AlGaN-related deep levels do not contribute to these spectra either, suggesting that the deep level onsets near 1.5, 2.7, and 3.3 eV occurring at both accumulation and pinch-off derive from the GaN region.

Precise deep level energies were obtained from C-DLOS. Figure 1(b) compares the C-DLOS spectra for V_G=0 and −3.6 V bias conditions, which are offset for clarity. The spectrum corresponding to V_G=−4 V (not shown) was similar to that of V_G=−3.6 V. The solid lines are theoretical fits determining the relevant parameters E^o and $d_{\rm FC}$. The model of Lucovsky[9] was used to fit the sharper σ^o without consideration of lattice relaxation effects, while the model of Chantre *et al.*[7] was applied for the broad spectra requiring inclusion of $d_{\rm FC}$ for a good fit. For the model of Chantre *et al.*,[7] fitted E^o and $d_{\rm FC}$ values were insensitive to interplay between other parameters. All onsets were positive, so E^o values were referred to E_c in this *n*-type structure. A deep level position of $E_c-3.85$ eV was determined for the AlGaN-related 3.9 eV onset. For the deep levels giving rise to the 2.7 eV onsets in accumulation and depletion SSPC spectra, similar σ^o spectra were found yielding E^o values of 2.63 and 2.65 eV at V_G=0 and −3.6 V, respectively, suggesting that these band gap states are identical. The discrepancy in E^o is attributed to the uncertainty in the data and the fitting procedure. Such arguments can also be made concerning the $E_c-3.30$ eV and $E_c-3.31$ eV levels associated with the

3.3 eV SSPC onsets at $V_G=0$ and −3.6 V, respectively. Henceforth, these states are assigned at $E_c-2.64$ eV and $E_c-3.30$ eV. DLOS analysis reveals that the 1.5 eV SSPC onsets apparent for $V_G=0$ and −3.6 V actually arise from different band gap states at $E_c-2.00$ eV with $d_{FC}=1.2$ eV (0 V) and $E_c-2.42$ eV with $d_{FC}=1.3$ eV (−3.6 V). The discrepancies between the SSPC threshold and E^o energies of these deep levels are a consequence of significant lattice relaxation as indicated by their large d_{FC}.

C-DLOS offers insight into the location of the observed deep levels. The $E_c-3.85$ eV band gap state is likely associated with either the Ni–AlGaN interface or the AlGaN barrier region. A distinction between these possibilities might be made by changing the Schottky metal. An AlGaN-related trap lying near E_v has been suggested by Meneghesso *et al.* based on I-DLTS investigation of an AlGaN/GaN HFET, although in that case the defect was attributed to the bare AlGaN surface.[2] Observation of the $E_c-2.42$, 2.64, and 3.30 eV deep levels at $V_G=-3.6$ V strongly implies that they are associated with either the UID-GaN or GaN:Fe regions, or both. Ascribing the $E_c-2.64$ eV level with MOCVD GaN agrees with a previous C-DLOS and DLTS study of *n*-type GaN grown by MOCVD that observed a band gap state at $E_v+0.87$ eV/$E_c-2.64$ eV,[11] for which gallium vacancy-related defects were identified as a likely source. Similarly, a PICTS investigation of a MOCVD-grown GaN metal-semiconductor field effect transistor reported a deep level at $E_c-2.67$ eV.[6] As with the $E_c-3.85$ eV state, the $E_c-2.00$ eV deep level was observed only for $V_G=0$ V and thus is attributed to the AlGaN cap. The $E_c-2.42$ eV state likely arises from the GaN region because it was evident only for $V_G=-3.6$ V, and its apparent absence at $V_G=0$ V can be explained by the overwhelming photoresponse of the $E_c-2.00$ eV deep level.

The increase of n_s due to deep level photoemission was estimated from lighted capacitance-voltage[12] (LCV) curves. The LCV curves were recorded by illuminating the diode with monochromatic light until the photocapacitance reached steady state and then performing a *C-V* scan while maintaining illumination. As is evident from the LCV scan in Fig. 2, at $h\nu=3.36$ eV photoemission increases n_s and thereby the capacitance, shifting V_{th} to a more negative value. In the same manner that *C-V* scans can determine n_s, the integrated increase in capacitance with illumination $\Delta C(V_G)$ (shown in the inset of Fig. 2) yields $\Delta n_s \geqslant 8.8\times 10^{10}$ cm^{-2}, which is primarily due to photoemission from the $E_c-2.64$ and 3.30 eV deep levels, though the $E_c-2.0$ eV and $E_c-2.4$ eV band gap states also contribute. From charge control of the 2DEG, $\Delta n_s=D_t$ only if the defects reside at the AlGaN surface or heterointerface, otherwise $\Delta n_s<D_t$.[3] Here, the distributions of AlGaN and GaN defects are unknown, so Δn_s must be considered to underestimate D_t. Also, optical excitation with $h\nu>E_g/2$ provides a lower bound for Δn_s because competing electron and hole photoemission from the same state is possible.[13] Determing Δn_s for the $E_c-3.85$ eV deep level proved problematic because the enhanced electric field in the AlGaN layer at reverse bias necessary for LCV caused additional redshifting of the AlGaN band edge via the Franz-Keldysh effect such that electron-hole pair creation became indistinct from photoemission from the $E_c-3.85$ eV deep level. This could be remedied with a simple test structure requiring low applied bias such as Ohmic pads separated by a semitransparent Ni field, where the proportional increase with illumination of the conductance between the pads and that of n_s are approximately equal. In any case, this result suggests that deep levels in the GaN buffer would appreciably diminish the maximum drain current in a HFET device since $\Delta n_s(h\nu=3.36$ eV) is, at minimum, ~1.5% of $n_s=6.2\times 10^{12}$ cm^{-2}. Due to their deep position relative to E_c, the deep levels attributed to the GaN region are unlikely to be involved in high frequency dispersion; however, the $E_c-3.85$ eV AlGaN level could induce dispersion in cases where E_F approaches E_v.

In summary, deep levels observed via C-DLOS in an AlGaN/GaN heterostructure equivalent to a HFET were associated with either AlGaN or GaN regions by comparing C-DLOS spectra at both accumulation and pinch-off. This effectively accomplishes trap depth profiling from the AlGaN barrier through the GaN bulk regions under the “gate” contact. Using LCV the influence of deep levels in the GaN on n_s was estimated.

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