Simulation of Deep-Level Trap Distributions in AlGaN/GaN HEMTs and Its Influence on Transient Analysis of Drain Current

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AlGaN/GaN high electron mobility transistors for high efficiency power switching applications are susceptible to charge trapping by deep-levels in the GaN buffer resulting in current collapse during gate and drain voltage swings. Although drain-current transient based methodologies have been used consistently to extract trap parameters, the factors affecting the non-exponential nature of the transient are still not well understood. No effort at accurately replicating multiple deep-levels in the GaN buffer to simulate transient response of GaN based power devices has been reported previously. In this work, we present numerical simulation results of HEMTs having multiple discrete trap states as well as band-like distribution of traps in the GaN band-gap. On-state current of synchronous gate and drain pulsed simulations show current as a sum of stretched multieponentials, with stretching factor showing trap and Fermi-level dependence. Using this capability incorporated into FLOODS TCAD simulator and definition of deep-levels in the GaN buffer precisely, modeling of non-exponential transients and associated wide peaks in the transient derivatives can be carried out accurately.

GaN based High Electron Mobility Transistors (HEMT)s, which leverage wide-band-gap related properties, are established as ideal candidates for high-power, high-efficiency and high-frequency applications ranging from RF communication to power conversion. However, the most unremitting technological challenge limiting the wide-spread adoption of GaN process technology is understanding and predicting their reliability and degradation modes therein. Many concur that most of the reliability-limiting mechanisms and issues are related to the presence of defect states in the forbidden band-gap of GaN, and the subsequent performance degradation associated with such defects.

Drain-current transient analysis experiments have helped shed light on the degradation observed in switching performance, often manifesting in AlGaN/GaN HEMTs as gate lag, drain lag and current collapse. The collapse is attributed to electron trapping comprised of lateral and vertical components. The lateral component due to tunneling of electrons from the gate to surface states at the AlGaN/GaN interface is facilitated by large bias difference between the gate and drain (under off-state and high drain bias). This phenomenon has been observed to be suppressed by improved passivation techniques. Under similar bias conditions, a vertical trapping component, which deteriorates dynamic performance, dominates in devices with improves passivation. The mechanism is expected to involve injection of 2DEG electrons deeper into the buffer and consequent trapping for several buffer designs. If the traps directly underneath the gate dominate, a shift in dynamic threshold is observed. However, if the traps in the drain access region dominate, they end up depleting the 2DEG in this region thereby increasing the dynamic on-resistance.

Much of experimental work identifying GaN buffer traps responsible for deterioration of dynamic performance utilize thermal dependence of the relaxation time constants to extract trap activation energy. Current relaxation time constants are obtained by taking the derivative of such transients and typically indicate the presence of multiple trapping centers. The extracted derivatives assume an asymmetric shape, with a long tail to the left and a broad peak indicative of a stretched multieponential transition instead of a pure exponential. While such a stretching factor has been associated commonly with deep-level traps, the exact physical mechanisms influencing the extended nature of exponential transition are not well understood.

Two-dimensional numerical simulations of AlGaN/GaN HEMTs have often been used to comprehend the role of buffer traps in current collapse. Dynamic I-V relationships extracted through such simulation results have shown good agreement with experimentally observed current collapse for GaN devices with different buffer doping schemes. However, no attempt to precisely capture the current relaxation behavior observed during transient analysis has been reported to the author’s best knowledge. TCAD modeling efforts using commercial tools at replicating transient behavior of unintentionally doped GaN (UID-GaN) generally adopt the three-level compensation model. In this model, the transient aspect is contributed only by a single deep donor.

The introduction of a single discrete deep-level, while being sufficient to qualitatively simulate dynamic I-V curves and bias dependence of trap occupancy in the bulk, cannot successfully replicate current relaxation curves observed during transient analysis. To this end, introduction of multiple deep trap levels will be necessary to obtain curves with multiple relaxation time constants observed in experiments. However, this alone will not be sufficient to accurately replicate the GaN buffer. More recently, non-exponential nature of transients has been attributed to the presence of band-like distribution of trap states in the GaN band-gap. This work presents and discusses in detail, using FLOODS TCAD, how factors associated with defect distribution in the band-gap can individually affect the nature of the drain-current transient response. To the author’s knowledge, very few works have discussed multiple trap levels in a TCAD framework and none have considered establishing a comprehensive understanding of how different trap parameters can influence the nature of transients. In the first section, the impact of energy-level of a single deep donor on transient response is discussed. The effect is presented in terms of magnitude of current collapse and derivative of the current transient. In the second section, a multi-level scheme is introduced and impact of relevant trap parameters on the current transient is presented. In the last section, the effect of a band-like distribution of trap states in energy, as opposed to a discrete trap level, on the current transient is presented.

Simulation Methodology

The vertical stack of the HEMT device structure that has been simulated consists of 0.1 μm gate and passivation (silicon nitride), 20 nm AlGaN on 2 μm of unintentionally-doped (UID)-GaN buffer and 1 μm SiC substrate. Gate length is 0.3 μm, with 0.5 μm separation

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from source and 1 μm of separation from drain. AlGaN is defined with an Al mole fraction of 25%. The metal gate is simulated with a Schottky barrier height of 0.7 eV, while the ohmic contacts at the source and drain are implemented by introducing high n-type doping. Fig. 1 shows a schematic of the device simulated with the trapping mechanism observed. Under off-state bias, 2DEG carriers are expected to be injected deeper into the substrate, thus getting trapped by the unoccupied traps underneath the gate as well as those in the drain access region. For replicating carrier transport for the selected device the unoccupied traps are implemented by introducing high n-type doping. The metal gate is simulated with an Al mole fraction of 25%. The ohmic contacts at the source and drain are simulated using Florida Object Oriented Device Simulator (FLOODS) TCAD simulator. FLOODS is a finite-element solver which solves the coupled partial differential equations in the form of Poisson’s Equation 1, continuity Equation 2 and current density (3) for electrons and holes, to simulate electrical behavior of the defined device.

\[
\nabla^2 \psi = -\frac{q}{\epsilon} \left[ p - n + N_D^+ - N_A^- \right] \\
\frac{\partial n}{\partial t} = \frac{1}{q} \nabla J_n, \quad \frac{\partial p}{\partial t} = \frac{1}{q} \nabla J_p \\
J_n = -q\mu_n n \nabla \phi_{fn} \quad J_p = q\mu_p p \nabla \phi_{fp},
\]

where \( \psi \) is electrostatic potential, \( p \) and \( n \) are hole and electron concentrations respectively, \( N_D^+ \) and \( N_A^- \) are ionized donor and acceptor-like impurities respectively, \( \epsilon \) is material permittivity, \( \mu_n \) and \( \mu_p \) are the carrier mobilities, and \( \phi_{fn} \) and \( \phi_{fp} \) are quasi-Fermi-levels for the respective carriers.

In order to introduce the dynamic nature of capture and emission processes associated with deep level traps, rate equations are introduced with carrier capture and emission rates defined as per Shockley-Read-Hall statistics:

\[
\frac{\partial n}{\partial t} = \frac{1}{q} \nabla J_n - c_n n N_D^+ + e_a (N_D - N_D^+), \\
\frac{\partial N_D^+}{\partial t} = -c_n n N_D^+ + e_a (N_D - N_D^+), \\
e_a = \frac{1}{\tau}, \quad c_n = \frac{e_n}{2N_c} \exp \left( \frac{E_c - E_T}{kT} \right),
\]

where the deep-level is defined through parameters \( N_0 \) (total concentration), \( E_c - E_T \), which is trap energy-level with respect to conduction band for donor-like trap, and \( \tau \) as emission time constant (alternative to capture cross-section).

Since the HEMTs simulated are depletion mode devices, complete pinch off under negative gate bias requires selection of the appropriate substrate charge. Most TCAD simulation work in literature achieve this by implementing the three-level compensation model. In this model, known donor impurities such as Silicon and Oxygen are introduced as fixed background doping, while Carbon and other acceptor-like defects are introduced at approximately 0.9 eV above the valence band. The shallow donor impurity is introduced at concentration of \( 10^{15} \text{cm}^{-3} \) and the deep acceptor at a concentration of \( 5 \times 10^{16} \text{cm}^{-3} \).

Several defect characterization efforts have determined the Fermi-level to be pinned in the upper half of the GaN band-gap. The three-level compensation model achieves Fermi-level pinning by introducing a deep donor-like trap level in the upper-half of the band-gap that also contributes to the observed transient response. With a deep-level donor concentration of \( 10^{17} \text{cm}^{-3} \) that is higher than the acceptor concentration, the Fermi-level gets pinned at the donor level to maintain charge neutrality in the bulk. Fig. 2 shows the GaN buffer defect model that has been modified to implement the multi-level traps and Gaussian-broadening of the deep donor level.

Transient simulations carried out consist of an initial off-state quasi-steady drain stress \( V_{GSO} = -5V \) followed by the on-pulse \( (V_{GS} = 0V \text{, } V_{DS} = 5V) \) during which the nature of the drain current transient will be observed. The drain stress during the off-state is less compared to that typically used for dynamic I-V measurements. However, the small dimension of the gate-to-drain access region allows sufficient depletion of electrons from the two-dimensional electron gas (2DEG), resulting in moderate current collapse.

### Results and Discussion

**Energy-Level dependence.**—In the three-level compensation model, a single discrete-trap level serves as a simplified model to understand the current collapse mechanism. The deep donor-trap level in GaN is generally introduced approximately 1 eV below the conduction band.\(^{21}\) We first expand results of this model by simulating the dependence of the transient behavior on the donor-trap energy level. Fig. 3a presents the impact of variation of the deep donor levels \( E_c = -0.4 \text{ eV to } E_c = -2.0 \text{ eV} \). Extent of current collapse and transient response was compared by normalizing drain current to the final steady-state value. Devices with deeper traps are expected to exhibit lower current as the Fermi-level gets pinned deeper in the band-gap. Also, deeper traps are slowest to recover to steady-state as one might expect according to slower emission rates, as shown in Fig. 3a. However, the normalized magnitude of current collapse has a U-shaped dependence on the deep-donor level, with traps having
activation energy in the range of 0.7 eV–1.3 eV showing maximum current collapse.

Transition in substrate charge integrated vertically along a slice in the drain access region (50 nm to the right of drain-side gate edge) was normalized and compared in Fig. 3b. The U-shaped dependence on trap-level can then be explained as follows. For a trap that is shallow, the tendency to trap electrons is too small to significantly deplete the 2DEG, as per SRH relation of capture and emission rates. On the other hand, if the trap happens to be too deep to trap electrons, the Fermi-level will no longer be pinned at a particular trap level and this can be expected to affect the nature of the transient to some extent.

Multi-level traps.—Results discussed in the previous section simulated the fundamental three-level compensation where the Fermi-level is pinned to the deep donor level. However, scenarios can arise where instead of a single dominant trap level, multiple trap levels having comparable defect densities might be present in the band-gap. As a consequence, the Fermi-level will no longer be pinned at a particular trap level and this can be expected to affect the nature of the exponential transient.

To observe the effect of variation of relative position of the Fermi-level with respect to the trapping state of interest, the deep donor has been split into two levels with equal concentrations, \( N_{DD1} \) and \( N_{DD2} \), of \( 5 \times 10^{16} \) cm\(^{-3} \). The shallower of the two donor-levels is maintained at \( E_C–1.0 \) eV while the deeper donor-levels is maintained at \( E_C–1.3 \) eV, which is an asymmetric peak with a longer tail to the left. For stretched exponential transient characterized by \( \beta < 1 \), Equation 2 represents an asymmetric peak with its amplitude reduced by the stretching factor, while the full width at half maximum (FWHM) of the peak is widened by the same factor.

Fig. 4 shows the derivative for transients obtained from donor traps at varying depths. As we go from shallower to deeper traps, stretching factor appears to exhibit an even more prominent U-shaped dependence on trap-level, similar to current collapse. In Fig. 3, shallowest and deepest traps at \( E_C–0.4 \) eV and \( E_C–2 \) eV respectively show purely exponential transition unlike the traps at \( E_C–1 \) eV. To get a better understanding, the transient derivative was observed by introducing the deep donor trap at different energy levels. The variation in the stretching factor of the exponential behavior can be observed in Fig. 4 as trap level at \( E_C–1 \) eV exhibits the most discernible extended exponential transition with \( \beta \) of 0.55, and traps exhibiting stretched exponentials between \( E_C–0.7 \) eV to \( E_C–1.3 \) eV. The relaxation time-constant, \( \tau_{\alpha} \), is determined by the position of the peak. It must be noted that the capture cross-section has been defined the same for all levels, corresponding to an emission time-constant, \( \tau_e \), of 1 second. Variation of the emission time-constant is expected to shift the current relaxation time-constant as well as affect the nature of the transient to some extent.

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emission time-constants. Once again, for both trap-levels, emission time $\tau$ is defined as 1 second.

Despite defining two trap levels, the current relaxation curves exhibit transients associated with only one trap, as shown in Fig. 5a. The observed transition is associated with just the shallower of the two deep traps. Since the two levels are defined with equal concentrations, the Fermi-level is now pinned between them, leaving the deeper trap completely occupied throughout the transient. To compare the nature of the transient, their derivatives have also been extracted and compared in Fig. 5b. For the device in which the two deep levels are separated by only 10 meV, the observed transient is almost identical to a single discrete level with concentration equal to their sum.

By defining the second trap deeper in the band-gap, the occupancy of the shallower trap can be expected to be increased. The resulting influence on the transient is visible in the form of a shift in the relaxation time-constant as well as lowering and widening of the derivative peak. These changes however appear to saturate beyond separation of the two deep levels exceeding 0.1 eV.

The examples discussed above exhibit just a single peak in the derivative, resulting from the participation of just the shallower of the deep traps. Transient analysis experiments typically indicate participation of multiple traps. To allow multiple trap levels to contribute to the transient behavior, another implementation of multiple trap levels was carried out by introducing three deep donor levels, with concentrations $N_{DD1}$, $N_{DD2}$ and $N_{DD3}$ of $2 \times 10^{16}$ cm$^{-3}$ each, and activation energy of 1 eV, 1.1 eV and 1.2 eV, respectively. A lower defect density and close spacing in energy allows transients associated with all the donor levels.

Figure 5. (a) Current transient and (b) derivative with log of time for second donor trap defined at different energy levels. Stretching factors are indicated with corresponding colors.

Figure 6. (a) Current transient and (b) derivative with logarithm of time for three deep donors defined in the GaN buffer. In (b), inset indicates transition (Previous: dot, Current: line) in donor ionization below the gate at different times for shallow (Red), mid-level (Black) and deep (Blue) traps.
Fig. 6 shows the drain current transient and its derivative in log of time. Participation of the three deep donor levels in the transient can also be confirmed from the extracted derivative exhibiting three distinct peaks. From the transient derivative, it can also be concluded that different trap levels appear to exhibit different stretching factors. Such a transient behavior can then be best described by a sum of stretched exponentials:

\[ I(t) = I_0 - \sum_{i} A_i e^{\left(-\frac{t}{\tau_i}\right)^\beta} \]  

where subscript \( i \) represents contributions from individual trap levels.

The most prominent peak associated with the shallowest deep donor (E\(_{\text{C}}\)−1 eV) exhibits almost no stretching (\( \beta = 1 \)), unlike the example with a single donor trap at E\(_{\text{C}}\)−1 eV (\( \beta = 0.55 \)). This example thus shows the relevance of the Fermi-level in determining the overall dynamics of carrier capture and emission. It also represents the complexity of the problem in determining the factors affecting the current relaxation behavior and the necessity of establishing a TCAD simulation framework capable of simulating multiple trap states accurately.

Definition of traps with equivalent concentrations allowed their respective derivative peaks to be prominent. If the concentrations of certain defect levels are still in the same order but lower than the trap exhibiting the dominant peak in the derivative, the overlapping of the peaks can result in a single wide peak, and hence a multieponential transition with closely spaced relaxation time-constants is expected.

**Gaussian-Broadening.**—Polyakov et al.\(^{22}\) have proposed the possibility of band-like distribution of defect states in the band-gap, as opposed to a discrete energy level, that can contribute to widening of the peak observed in the current transients. Such a band of defect states are expected to be distributed around a peak energy level E\(_{\text{C}}\). Initial considerations assume the density of such defect states to be distributed in a Gaussian or parabolic form around E\(_{\text{C}}\). Unlike the stretching factor contributing to the peak widening associated with single discrete defects, presence of a defect band can result in a transient best described by a sum of stretched multi-exponentials (Equation 3). The resulting widening of the peak is not just from stretching associated with individual trap levels, but also a result of the overlapping of the individual peaks.

Similar to multiple trap levels defined in the section on multiple trap levels, a Gaussian-like band has been defined in FLOODS represented by a finite number of discrete trap levels distributed in energy and concentration using rate equations. For a simple comparison, examples discussed involve three levels defining the Gaussian band, with the second level at E\(_{\text{C}}\)−1.0 eV representing the peak at E\(_{\text{C}}\).

In order to study the effect of a Gaussian spread in energy, four devices have been compared. All the devices implement the three-level compensation model, with deep donor at E\(_{\text{C}}\)−1.0 eV participating in the trapping dynamics. The first device with an extremely narrow FWHM of 0.01 eV has an almost “discrete” description, hence identical results to the case discussed in the section on single deep levels are expected. The other three HEMTs have the Gaussian broadening of the deep donor defined with a FWHM of 0.05 eV, 0.1 eV and 0.2 eV respectively.

Fig. 7a shows the current transient response to dynamic switching for all the four cases. Closer inspection of the transients requires comparison of their derivatives (Fig. 7b). A clear shift in the current relaxation time constant peak is observed with increasing FWHM. A marginal increase in current and faster transition with increasing FWHM can be attributed to upper half of the band becoming shallower. For FWHM of 0.05 eV and 0.1 eV, the derivative has a lower and considerably wider peak, indicating a more uniform de-trapping process as compared to the discrete definition. For FWHM of 0.2 eV, the description of the Gaussian by finite energy levels has become evident with larger spacing in energy between the trap levels. A multi-level like transition is observed with multiple peaks, with the peak associated with the shallower trap level becoming more prominent. This indicates a change in stretching factor for different trap levels with varying FWHM.

The examples presented are very specific as the Fermi-level is expected to be pinned at the mid-level of the defined deep donor distribution. The resulting transient after bias switching may not have identical exponential nature if the Fermi-level pinning is not observed, as was the case in the multi-level trap examples.

**Discussion**

The three-level compensation model is insufficient to capture the bias switching-related trap dynamics accurately due to presence of multiple trap levels in the GaN band-gap. By extending the three-level compensation model to portray such practical scenarios, modeling of transient behavior and factors affecting the nature of such transients can be carried out more accurately.

Incorporating the ability to model multiple trap states in the GaN buffer allows simulation of scenarios where multiple peaks in the current relaxation derivative is observed. However, trap parameters extracted by transient methodology may not be sufficient as other traps not contributing to the transient behavior will play a significant role in determining the Fermi-level, and consequently the simulated transient itself. Incorporation of defect characterization techniques capable of...
extracting trap parameters related to all the defect levels encountered in the GaN band-gap will be necessary.24–27 An accurate modeling of current relaxation curves, and consequently current collapse behavior thus entails comprehensive integration of all the tools in addition to TCAD simulation capability.

Conclusions

TCAD simulation of switched-biasing transient-analysis experiments was carried out to observe the impact of deep-level traps in the GaN buffer. Parameters influencing the distribution of multiple trap states in the GaN band-gap were varied. Drain current transients thus obtained were investigated by extracting their derivatives with logarithm of time and comparing among different cases. For peaks associated with individual trap levels, the stretching factor was observed to be dependent on the relative position of the trap and Fermi-level. Transients associated with multiple trap states exhibited transient behavior best described by a sum of stretched multiexponentials, where the stretching factor once again showed variation with defects at different energy levels. By implementing a Gaussian band-like distribution of defect states in energy, transients characterized by a single wide peak was observed, which can be described by multiple stretched exponentials with closely spaced relaxation time constants. Varying FWHM of the band-like distribution exhibits change in the stretching factor associated with each segment of the band. Improved understanding of the factors responsible for affecting stretching factor will help achieve better fits to experimental results. The combination of discrete multilevel and band-like density of defect states can thus be utilized to most accurately model HEMTs showing transient derivative with multiple peaks.

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