

Physics-Informed Compact Modeling of Off-State Leakage and Breakdown in GaN-on-Si Devices

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Abstract—Atomera’s oxygen-insertion (OI) technology, referred to as Mears Silicon Technology (MST), introduces partial oxygen-containing monolayers into Si during epitaxy, altering near-surface intermixing and nitride nucleation. This work uses off-state I_D - V_D leakage data from GaN-on-Si high-electron-mobility transistor (HEMT) test structures to examine how MST changes the GaN-on-Si electrical behavior. A compact leakage model is developed for three wafer splits: a Czochralski-grown (CZ) control wafer, an MST/OI split, and a high-resistivity Si (HR-Si) reference. The model treats the off-state current as a bias-quenched low-bias parasitic branch plus a variable-range-hopping (VRH)-inspired activated leakage path whose coupling to a buried AlN/Si-related parasitic channel is limited by a finite current ceiling; the high-field rise is represented by distributed soft breakdown. Supporting spreading resistance probe (SRP) data show reduced active carrier concentration near the buried AlN/Si-side region for an MST-containing GaN/AlN stack. The MST/OI split shows reduced leakage and delayed high-field current rise relative to the CZ control, while differing from the HR-Si benchmark. These trends support an interface-first picture in which MST modifies the buried AlN/Si-related leakage path rather than acting only through bulk substrate resistivity.

Keywords— Mears Silicon Technology, GaN-on-Si, HEMT, compact modeling, leakage, breakdown, AlN/Si interface, oxygen insertion

I. INTRODUCTION

Insertion of partial oxygen-containing monolayers during Si epitaxy produces local changes in bonding, lattice distortion, and near-surface intermixing behavior [1], [2]. In prior Si complementary metal-oxide-semiconductor (CMOS) work, MST layers have been shown to suppress oxidation-enhanced boron diffusion [1] and improve gate-dielectric reliability [2]. For the present GaN-on-Si problem, MST, as sketched in Fig. 1(a), is an atomically thin Si-side perturbation located in the near-surface Si region immediately below the nitride nucleation layer, exactly where the AlN nucleation chemistry and Si/nitride intermixing are established.

GaN-on-Si remains attractive for large-area, lower-cost power devices [3], but its off-state performance is strongly influenced by the buried AlN/Si region. Substrate nitridation can suppress Al diffusion into Si [4]. Three-terminal breakdown studies identify the AlN/Si region as a contributor to premature off-state breakdown and show that a SiN_x

interlayer can improve leakage and breakdown characteristics [5]. RF studies on GaN-on-Si point to a parasitic conductive

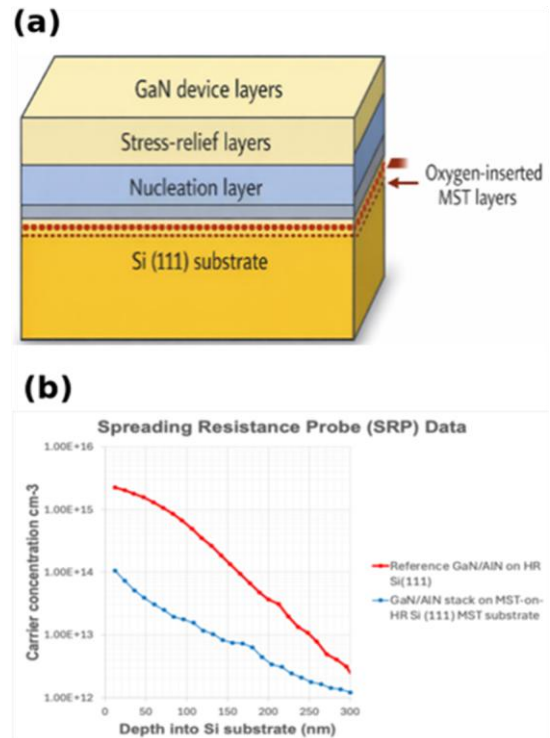


Fig. 1. Physical location and materials-level evidence for MST/OI in GaN-on-Si. (a) Generalized epitaxial structure showing oxygen-inserted MST layers in the near-surface Si(111) region, immediately below the nitride nucleation layer. (b) Spreading resistance probe (SRP) comparison, showing reduced active carrier concentration for the MST/OI-containing GaN/AlN-on-Si structure. The SRP trend is used as qualitative support for a modified buried Si/AlN-side electrical environment, not as a direct fit constraint.

interfacial sheet as an important source of RF loss [6]. A high-resistivity starting substrate therefore does not by itself remove the buried-interface problem; active charge or a parasitic sheet can still be created during nitride nucleation and growth. Defect-assisted leakage also remains highly relevant in GaN devices [7]–[10].

Although the HEMT channel is near the surface, high drain bias can extend field lines and defect-assisted leakage paths through the buffer to the buried AlN/Si-related region. Thus, a surface device can be affected by a buried path without requiring the conducting channel itself to reside at the interface.

Experimentally, MST-modified GaN-on-Si wafers show systematic changes in off-state I_D - V_D leakage. Relative to the CZ control, the MST/OI split has a smaller low-bias shoulder, lower intermediate-voltage leakage, and delayed high-field current rise. The HR-Si benchmark lowers leakage but does not reproduce the same full curve evolution, indicating that the MST effect is not described only by higher bulk substrate resistivity. A second MST-on-CZ split shows the same qualitative trend.

These experimental trends motivate the compact-model analysis. Rather than comparing only single-voltage leakage values or apparent breakdown voltages, we ask whether the full I_D - V_D curve evolution can be decomposed into a compact set of physically interpretable terms that change systematically with MST/OI. The same model form is applied to the CZ control, MST/OI, and HR-Si splits, treating the low-bias shoulder, intermediate-current ceiling, and high-field rise as separate electrical contributions. This lets the MST/OI effect be discussed in terms of changes to a buried AlN/Si-related leakage path and nearby buffer/defect-assisted access, without assigning a unique microscopic trajectory to every carrier.

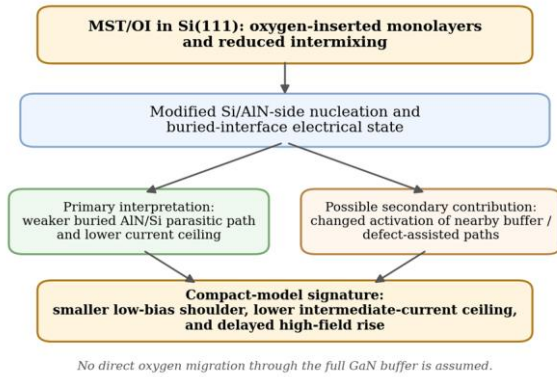


Fig. 2. Working hypothesis connecting MST/OI process modification to the compact leakage model. MST/OI is treated as a Si-side perturbation of the nucleation and buried-interface region. The compact-model signature is a smaller low-bias shoulder, lower intermediate-current ceiling, and delayed high-field rise.

The working hypothesis, summarized in Fig. 2, is interface-first: MST may change the AlN nucleation or buried AlN/Si-side boundary condition, weakening a parasitic buried path. Nearby defect-assisted participation is not excluded, and no direct oxygen migration through the full GaN buffer is assumed. Supporting SRP data in Fig. 1(b) provide a qualitative materials-level check on this interpretation: in a related GaN/AlN-on-Si comparison, the MST-containing stack shows reduced active-carrier concentration near the buried AlN/Si-side region. Because SRP senses electrically active charge rather than total elemental concentration, this result bears directly on the leakage picture and is consistent with MST/OI reducing the active parasitic charge associated with the buried interface. The SRP samples are not a matched version of the HEMT electrical splits, so the SRP data are not used as fit constraints.

II. EXPERIMENTAL DATA SET

The electrical data set was chosen to separate three effects: the MST/OI process change, the role of starting Si substrate, and geometry dependence. Off-state I_D - V_D sweeps were measured at $V_G = -4$ V on lateral GaN-on-Si HEMT test structures. The main GD3 comparison uses $L_{GD} = 3$ μ m devices from CZ control, MST/OI, and HR-Si splits. GD8 devices with $L_{GD} = 8$ μ m provide a geometry check, while a second MST/OI-on-CZ split supports reproducibility.

The GD3 medians show the three features modeled below: a reproducible low-bias shoulder, reduced MST/OI intermediate-current level, and delayed high-field rise relative to the CZ control. HR-Si lowers leakage but does not reproduce the same intermediate-current behavior or GD8/GD3 response, consistent with a distinction between bulk substrate resistivity and the Si/AlN-side boundary condition where parasitic charge is formed.

III. COMPACT MODEL

For one fixed layout the off-state current is written in the voltage domain rather than by treating V/L_{GD} as a microscopic local field. The local field in a lateral HEMT is highly nonuniform, and the present data do not justify assigning absolute microscopic meaning to a fitted field threshold. The compact form is

$$I_D(V) = I_{sh}(V) + M_{BD}(V)I_{path}(V), \quad (1)$$

where I_{sh} captures the low-bias shoulder and $M_{BD}I_{path}$ represents the high-field leakage and soft-breakdown response. The shoulder branch is written as

$$I_{sh}(V) = G_{sh}V \exp \left[- \left(\frac{V}{V_{sh}} \right)^q \right]. \quad (2)$$

It is linear at small voltage and is progressively quenched at larger voltage. Physically, this branch represents a weak low-bias parasitic path suppressed by trap charging, depletion, or carrier redistribution in the buried/interface-related leakage network. Its inclusion is not merely numerical: the non-monotonic shoulder is a reproducible feature of the measured curves and is difficult to reconcile with a single monotonic leakage branch.

The high-field path is represented by the harmonic mean of an activated branch and a buried-path current ceiling,

$$I_{path} = \frac{I_{act}I_b}{I_{act} + I_b}, \quad G_{path}^{-1} = G_{act}^{-1} + G_b^{-1} \quad (3)$$

$$I_{act} = VG_0 \exp \left[- \left(\frac{V_0}{V_a} \right)^{1/2} \right] \quad (4)$$

$$V_a = V_s \ln \left[1 + \exp \left(\frac{V - V_{th}}{V_s} \right) \right] \quad (5)$$

$$I_b = I_{ceil} \left[1 + \left(\frac{V_p}{V} \right)^p \right]^{-1} \quad (6)$$

Here I_{act} represents voltage-activated leakage through the GaN buffer, with threading dislocations and their associated trap states providing plausible leakage pathways. The $\exp [-(V_0/V_a)^{1/2}]$ curvature is VRH-inspired, following Efros-Shklovskii-like field-activated forms used in GaN leakage analysis. In this work, however, the term is used as a compact room-temperature representation of the pre-knee I_D - V_D curvature, not as proof of a unique VRH regime or of purely dislocation-core transport [8], [10]. The I_b term is a phenomenological current ceiling associated with the buried AlN/Si-related path. The soft-breakdown multiplier is

$$M_{BD}(V) = 1 + A\Phi_N\left(\frac{\ln V - \ln V_{br}}{\sigma_{ln}}\right)\left(\frac{V}{V_{br}}\right)^{m_{BD}}, \quad (7)$$

where Φ_N is the standard normal cumulative distribution. This term represents a distributed onset of rapid current rise, not necessarily a single avalanche event, the power-law factor sustains the post-onset rise

The model is not used to assign microscopic meaning to every fitted parameter. The robust information is the separation of curve features: I_{sh} captures the shoulder, I_b controls the intermediate-current ceiling, and M_{BD} controls the rapid high-field rise. Pre-knee shape parameters are partially correlated in a single-temperature voltage-domain fit, so the discussion emphasizes parameter groups and branch assignments rather than each auxiliary parameter independently.

IV. DATA FITS

The purpose of the fit is to determine whether the MST/OI-dependent changes in the measured I_D - V_D curves can be represented by a compact, physically interpretable parameter set. Table I reports the resulting model parameters, grouped by their role in the two-stage fit. The optimization is done in two stages. The stage-1 parameters define the monotonic compact leakage path and high-field onset, while the stage-2 parameters describe the low-bias shoulder and refine the leakage/break-down shape with the Stage-1 onset retained.

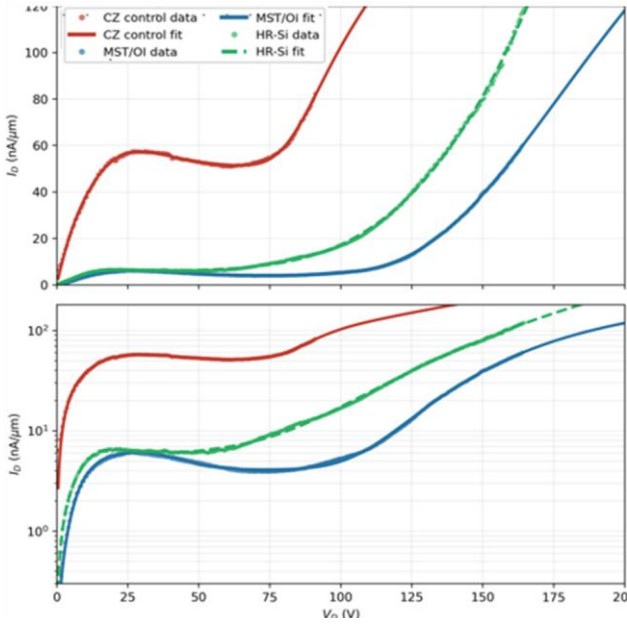


Fig. 3. GD3 median off-state I_D - V_D curves and compact-model fits. Markers show split medians; solid lines are the compact fits. The same data are shown on linear and logarithmic current scales.

Fig. 3 shows the GD3 median traces and the compact-model fits. The model captures the main observed features: the strong low-bias shoulder of the CZ control, the lower MST/OI intermediate leakage, and the delayed high-field rise of the MST/OI split relative to the CZ control and HR-Si benchmark.

The fitted shoulder amplitudes differ strongly between splits. The CZ control has a large low-bias shoulder, peaking near 49 nA/μm. The MST/OI and HR-Si shoulders are much smaller, near 2.5 nA/μm. This gives a physical meaning to the low-bias non-monotonicity: a buried or buffer-related path can initially participate in conduction and then be partially

quenched as drain bias changes the charge state and electrostatic boundary condition of the leakage network.

TABLE I. MODEL PARAMETERS.

Parameter	Units	Stage	CZ	MST	HR-Si
V_{th}	V	1	60	59.99	60
V_s	V	1	29.37	19.03	19.34
G_0	nA/μm/V	1	1000	1000	1000
V_p	V	1	1	1	42
p	-	1	0.9044	1.905	0.3
V_{br}	V	1	86.75	160.9	250
V_0	V	2	1	90.31	84.73
I_{ceil}	nA/μm	2	9.761	3.924	10.2
σ_{ln}	-	2	0.7766	0.2471	2
A	-	2	10.85	25.95	227.2
m_{BD}	-	2	2.404	2.016	3.907
G_{sh}	nA/μm/V	2	3.139	0.2254	0.5908
V_{sh}	V	2	38.97	26.78	12.3
q_{sh}	-	2	1.532	1.569	1.005
GD8/GD3	-	-	0.8	3.17	3.84

Fig. 4 decomposes the fits into shoulder, high-field path, and current-ceiling components. The decomposition is an electrical separation of measured curve features, not a unique microscopic trajectory. In this representation, MST/OI has a smaller low-bias shoulder, lower intermediate-current level, and later high-field rise than the CZ control. HR-Si also lowers leakage, but its high-field evolution differs from MST/OI, showing that starting-substrate resistivity alone is not the relevant control variable; the electrical state of the buried Si/AlN-side region after nitride growth also matters.

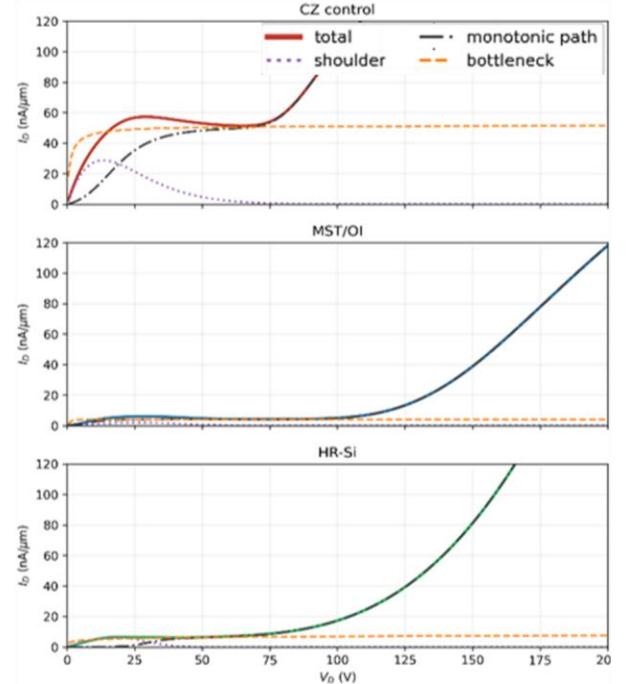


Fig. 4. Component decomposition of the compact fits. The shoulder term dominates the non-monotonic low-bias feature, while the high-field branch controls the later rapid rise.

V. GEOMETRY AND TRANSPORT SCREENING

GD8 data provide an external check on the GD3 interpretation. If a split is already limited by a buried-path current ceiling, changing L_{GD} should weakly affect the intermediate-current level. If the activated branch remains important, larger gate-drain spacing should change the current

more strongly. Experimentally, the GD8/GD3 intermediate-current ratio is near unity for the CZ control but increases strongly for MST/OI and HR-Si, as listed in Table I. This is consistent with the CZ control being closer to a parasitic-path-limited regime, while MST/OI and HR-Si remain more sensitive to voltage-domain activation and geometry.

The pre-knee transforms in Fig. 5 are used only as consistency checks for the activated branch. For the voltage-domain form used here, the VRH-inspired term $I_{\text{act}} = V_D G_0 \exp[-(V_0/V_a)^{1/2}]$ predicts that $\ln(I_D/V_D)$ should vary approximately linearly with $V_a^{-1/2}$, or with $V_D^{-1/2}$ when V_D is used as the effective drive voltage for a fixed device layout. A Poole-Frenkel-like form is instead screened by plotting $\ln(I_D/V_D)$ versus $V_D^{1/2}$. In the present room-temperature data, the MST/OI and HR-Si traces are more nearly linear in the VRH-inspired transform. This supports the activated-branch curvature used in the compact model, but it does not uniquely identify Efros-Shklovskii variable-range hopping, because the same voltage range also contains contributions from the low-bias shoulder and the buried-path ceiling. Temperature-dependent I - V and three-terminal substrate-current monitoring remain needed to discriminate among hopping, trap-assisted tunneling, Poole-Frenkel emission, and interface-sheet conduction.

VI. DISCUSSION

The shoulder term is required because the measured GD3

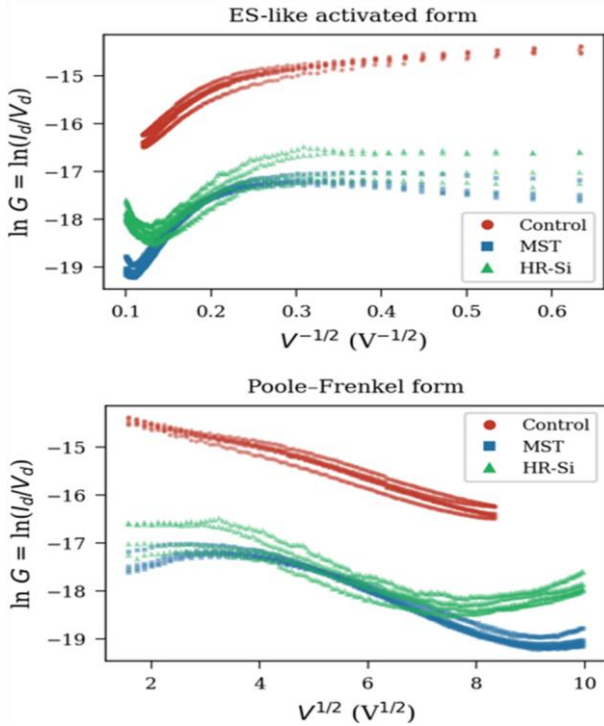


Fig. 5. Pre-knee screening transforms for the same GD3 data. Top: ES-like activated form, $\ln(I_D/V_D)$ versus $V_D^{-1/2}$. Bottom: Poole-Frenkel form, $\ln(I_D/V_D)$ versus $V_D^{1/2}$. The comparison is used as a screening diagnostic, not as proof of a unique microscopic transport law.

medians are non-monotonic at low bias. Adding I_{sh} prevents the low-bias shoulder from being incorrectly absorbed into I_{ceil} or V_{br} , allowing the high-field branch to describe the transition from activated leakage to buried-path limitation and soft breakdown.

The shoulder mechanism is not uniquely identified by the present room-temperature data. Possible origins include trap

charging in the buffer, depletion of a weak parasitic sheet, carrier redistribution near the buried AlN/Si path, or a combination of these. The same ambiguity is also why the HR-Si comparison is useful. HR-Si changes the bulk substrate resistivity, while MST/OI is placed at the Si-side boundary where nitride nucleation and interface charge formation occur. If the MST/OI effect were only an effective increase in substrate resistivity, the HR-Si traces would be expected to reproduce the same curve evolution. Instead, HR-Si lowers leakage but shows different high-field evolution and GD8/GD3 response. This supports the view that the relevant variable is the electrical state of the buried interface region after nitride growth, not only the resistivity of the starting Si wafer. Although Table I lists fitted compact-model parameters, not all should be interpreted with equal physical weight. The most robust conclusions come from parameter groups and curve-level behavior: the shoulder branch is smaller for MST/OI, the buried-path current ceiling is reduced, and the high-field rise is delayed relative to the CZ control. Internal shape parameters such as A , σ_{In} , and q_{sh} reproduce the curves but should not be treated as unique microscopic constants.

VII. CONCLUSION

This work develops a compact, two-stage leakage model that reproduces the non-monotonic off-state I_D - V_D behavior of GaN-on-Si HEMTs across CZ-control, MST/OI, and HR-Si splits. Its value is that it converts each curve into a small set of physically interpretable, directly comparable quantities and localizes the MST/OI effect to a specific part of the leakage. On this basis, MST/OI lowers off-state leakage and delays the high-field rise in a way that higher bulk substrate resistivity alone does not reproduce, pointing to a change in the buried AlN/Si-related leakage path. These quantities form a compact metric set for comparing process splits and tracking MST/OI changes beyond the ones studied here. Temperature-dependent I - V and three-terminal substrate-current measurements would further separate the candidate leakage mechanisms and sharpen the physical interpretation.

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