



Defect Engineering in Gallium Nitride Semiconductors for Improving Carrier Mobility and High-Power Electronic Device Reliability

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ABSTRACT :

Gallium nitride power devices increasingly operate at electric-field, switching-frequency, and junction-temperature regimes where defect-mediated carrier trapping becomes a principal constraint on transport stability and operational lifetime. This study investigates how targeted defect engineering can modify the relationship between GaN microstructure, electron mobility, and degradation in high-power electronic devices. The analysis focuses on nitrogen vacancies, gallium vacancies, carbon- and oxygen-related impurities, threading dislocations, and interface traps whose electronic states promote Coulomb scattering, carrier capture, dynamic on-resistance, leakage, and threshold-voltage instability. A defect–transport–reliability framework is developed to connect defect concentration and trap energetics with mobility degradation and electrically activated failure mechanisms. Engineering interventions including epitaxial growth-condition control, compensation management, dislocation reduction, interface passivation, and post-growth thermal processing are comparatively examined. Particular emphasis is placed on distinguishing defects that primarily limit channel transport from deep-level traps activated under high-field and high-temperature stress. The framework establishes measurable links among trap density, electron mobility, current collapse, leakage evolution, and device degradation, providing a pathway for optimizing GaN heterostructures for sustained high-voltage operation without sacrificing transport performance or switching efficiency.

Keywords: Gallium Nitride; Deep-Level Traps; Threading Dislocations; Carrier Mobility; Dynamic On-Resistance; Device Reliability

1. INTRODUCTION AND DEFECT–PERFORMANCE PROBLEM DEFINITION

1.1 GaN for High-Power Electronic Devices

Gallium nitride combines a wide bandgap, high critical electric field, and high electron saturation velocity, supporting high-field, high-temperature advanced power electronics [1]. In AlGaIn/GaN heterostructures, polarization creates a high-density two-dimensional electron gas (2DEG) that enables rapid transport and high-frequency switching. These properties offer low specific ON-resistance and high breakdown capability in GaN HEMTs and normally-off p-GaN gate devices [2]. Consequently, GaN supports efficient modern power conversion in chargers, renewable-energy converters, and electric-drive systems. Yet intrinsic advantages do not guarantee device reliability because material defects, interface states, and carrier trapping alter channel transport during realistic electrical and thermal operating stress [3].

1.2 Defect-Limited Carrier Transport

Carrier transport in practical GaN structures is strongly conditioned by electrically active imperfections. Nitrogen vacancies (V_N), gallium vacancies (V_{Ga}), substitutional impurities, carbon- and oxygen-related states, threading dislocations, interface traps, surface states, buffer traps, and gate-stack defects perturb channel charge and local device electrostatics [4]. Charged defects increase carrier scattering, while deep states capture and release carriers over field- and temperature-dependent timescales. These processes reduce effective channel mobility, promote recombination, shift threshold behaviour, and produce gate lag, drain lag, current collapse, and elevated dynamic R_{ON} [5]. Temperature-dependent transient measurements distinguish trapping contributions arising from surface/barrier and GaN buffer regions [6]. Deep-level characterization also indicates multiple active trap energies, making degradation dependent on defect location, occupancy, capture cross-section, and emission kinetics [7].

1.3 Defect Engineering as an Optimization Problem

Defect engineering should therefore be treated as a controlled optimization problem rather than simply minimizing total defect density. Variables include defect species, concentration, energetic position within the bandgap, spatial distribution, and charge state [8]. Growth temperature, epitaxial strain management, surface passivation, gate processing, and thermal treatments can reshape this defect landscape. These processing conditions determine the resulting defect population and associated trap kinetics, which subsequently influence carrier transport, electrical performance, and long-

term device reliability. Here, structural defects and electrically active traps become intermediate variables linking fabrication conditions to device behaviour [3]. Effective process optimization must suppress harmful scattering and slow trapping while preserving functions including buffer isolation, field control, and stable threshold operation [6].

1.4 Research Gap, Objectives and Contributions

Existing investigations often isolate relationships among crystalline defects, trap spectroscopy, carrier mobility, current collapse, or reliability degradation [5]. A unified framework treats these phenomena as connected stages of one device-physics problem. This study integrates structural characterization, defect measurements, transport analysis, and reliability assessment [1]. It quantifies GaN defect populations and constructs descriptors representing density, energy, location, and trapping kinetics. These descriptors are related to mobility, threshold voltage, dynamic R_0N , leakage, and degradation indicators [7]. Robust predictive computational models then estimate transport and reliability responses, identify influential defect/process variables, and optimize fabrication conditions [4]. Finally, untreated and defect-engineered devices are benchmarked through electrical stress measurements interpreted alongside recognized reliability-testing practices, establishing a reproducible route from defect control to device performance [2].

2. PHYSICAL FRAMEWORK OF GAN DEFECTS, CARRIER TRANSPORT AND RELIABILITY

2.1 Defect Taxonomy and Formation Mechanisms

GaN defects span several structural scales and exhibit distinct transport consequences [11]. Point defects include nitrogen vacancies (V_N), gallium vacancies (V_{Ga}), interstitials, and antisites, originating from nonstoichiometric growth, irradiation, or thermal processing. Carbon, oxygen, hydrogen, and dopant-associated complexes arise from precursors, substrates, ambient contamination, and intentional compensation [7]. Extended defects comprise threading screw, edge, and mixed dislocations produced largely by lattice and thermal-expansion mismatch during heteroepitaxy. AlGaIn/GaN, dielectric/GaN, surface, and gate-stack states additionally emerge from dangling bonds, processing damage, oxidation, and imperfect interfaces [14]. Their thermodynamic stability is described by

$$E_f(D^q) = E_{\text{tot}}(D^q) - E_{\text{tot}}(\text{bulk}) - \sum_i n_i \mu_i + q(E_F + E_{\text{VBM}}) + E_{\text{corr}}$$

where E_{tot} denotes total energies, n_i exchanged atoms, μ_i chemical potentials, q defect charge, E_F Fermi level, E_{VBM} valence-band maximum, and E_{corr} finite-size correction. Thus, chemical environment and Fermi-level position determine energetically favourable defects [9].

2.2 Trap Occupancy and Carrier Capture

Electrically active defects influence transport according to their occupancy and carrier-exchange kinetics. For a trap at energy E_t , equilibrium electron occupancy follows

$$f_t = \frac{1}{1 + g_t \exp[(E_t - E_F)/k_B T]}$$

where E_F is the Fermi level, g_t the degeneracy factor, k_B Boltzmann constant, and T absolute temperature [15]. Occupancy therefore increases as E_F approaches or exceeds E_t , while temperature broadens the transition between empty and occupied states. Carrier capture is characterized by

$$\tau_c = \frac{1}{\sigma_n v_{th} n}$$

where σ_n is electron capture cross-section, v_{th} thermal velocity, and n electron concentration [10]. Consequently, large cross-sections and high carrier densities shorten capture times. Bias- and temperature-dependent transient measurements can therefore associate observed current recovery times with particular trapping processes, helping distinguish rapidly responding interface states from slower deep traps within GaN buffer regions [12].

2.3 Carrier Mobility and Scattering

Carrier mobility provides a measurable link between the defect landscape and channel transport. Where the device geometry and capacitance model permit, effective field-effect mobility can be estimated from transfer characteristics as

$$\mu_{\text{eff}} = \frac{L}{WC_i V_{DS}} \frac{\partial I_D}{\partial V_G}$$

where L and W are channel dimensions, C_i is effective gate capacitance, and V_{DS} represents drain-source bias [8]. The transconductance term $\partial I_D / \partial V_G$ consequently reflects gate-controlled channel conduction. Multiple scattering mechanisms can be separated conceptually through

$$\frac{1}{\mu_{\text{eff}}} = \frac{1}{\mu_{\text{phonon}}} + \frac{1}{\mu_{\text{dis}}} + \frac{1}{\mu_{\text{imp}}} + \frac{1}{\mu_{\text{interface}}}$$

representing phonon, dislocation, ionized-impurity, and interface-related contributions [13]. Rather than attributing mobility loss generically to defects, this decomposition permits temperature, defect-density, and interface-quality measurements to identify dominant scattering channels [7]. It also provides a quantitative basis for determining whether processing improvements genuinely enhance transport.

2.4 Defect-to-Reliability Propagation

Defects influence reliability through coupled electrical and thermal mechanisms rather than a single degradation event. Electrically active states capture channel carriers during high-field operation, modifying local charge distributions and redistributing electric fields near interfaces, gate edges, and buffer regions [11]. Subsequent mobility and current reduction can appear as threshold-voltage instability, current collapse, leakage variation, and increased dynamic R_{ON} . Importantly, post-switching R_{ON} may substantially exceed its static DC value because trapped charge persists after the stressing condition is removed [15]. Repeated switching then combines trapping-induced conduction losses with self-heating and high-field stress, progressively modifying trap populations and vulnerable interfaces [9]. Accumulated degradation ultimately produces parametric instability or catastrophic device failure.

2.5 Research Hypotheses

The framework supports four experimentally testable hypotheses. H1: reducing electrically active defect density increases effective carrier mobility by decreasing trap-mediated and charged-defect scattering [10]. H2: electrically measured trap density predicts dynamic R_{ON} degradation more effectively than structural defect density alone. H3: optimized defect engineering simultaneously improves mobility and electrical-stress lifetime by controlling detrimental defect populations [14]. H4: multivariate descriptors combining defect density, energy, location, charge state, and capture kinetics provide stronger reliability prediction than isolated defect variables [12]. These hypotheses establish measurable relationships for subsequent characterization, modelling, optimization, and device-level validation.

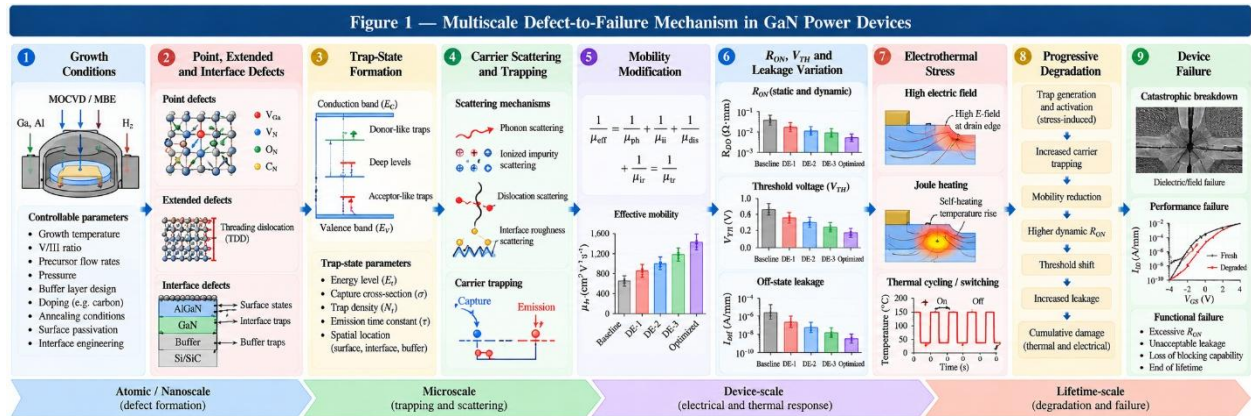


Figure 1 — Multiscale Defect-to-Failure Mechanism in GaN Power Devices

3. EXPERIMENTAL DESIGN, DATA ACQUISITION AND DEFECT ENGINEERING

3.1 Device and Sample Architecture

The experimental design comprises five matched sample groups: untreated baseline GaN, three progressively modified defect-engineering conditions (DE-1, DE-2, and DE-3), and an optimized condition selected from combined structural and electrical evidence [17]. Devices are fabricated from comparable AlGaN/GaN epitaxial structures using controlled barrier and buffer thicknesses, channel dimensions, gate geometry, metallization, and contact processes. Wafer position and device area are recorded to identify spatial variability [13]. Electrical characterization is performed using identical probe configurations, temperature, bias sequence, and stabilization periods. Replicate devices from each condition enable statistical comparison, ensuring that measured transport or reliability differences primarily reflect defect-engineering treatments rather than uncontrolled geometrical or processing variation [21].

3.2 Defect-Engineering Treatments

Defect populations are systematically modified through growth and post-growth processing variables selected for their influence on incorporation, compensation, interfaces, and trap formation. Controlled parameters include epitaxial growth temperature, V/III ratio, reactor pressure, buffer composition, carbon concentration, annealing temperature and duration, surface passivation, dielectric processing, and interface treatment [15]. Each condition varies predetermined factors while retaining comparable device fabrication. Optimization does not assume that minimum total defect concentration produces superior performance. Carbon incorporation in GaN buffers, for example, can improve resistivity, suppress parasitic conduction, and strengthen blocking behaviour, yet carbon-related deep states may increase carrier trapping and dynamic R_{ON} dispersion [24]. Likewise, aggressive thermal or surface treatments may remove particular states while generating interface damage elsewhere [18]. Treatment selection therefore balances

electrical isolation, trap kinetics, mobility, leakage, breakdown capability, and stability rather than optimizing a single defect metric.

3.3 Structural and Chemical Data Acquisition

Structural and chemical characterization establishes quantitative descriptors of each engineered defect landscape. High-resolution X-ray diffraction determines rocking-curve full width at half maximum (FWHM), providing indicators of crystalline mosaicity and dislocation-related disorder [14]. Cross-sectional and plan-view TEM/STEM quantify threading screw, edge, and mixed dislocation densities and identify localized structural imperfections. Atomic force microscopy measures surface root-mean-square roughness across multiple scan regions [20]. Secondary-ion mass spectrometry provides depth-resolved carbon, oxygen, and hydrogen concentrations through the barrier, channel, and buffer. Photoluminescence measurements record band-edge intensity, defect-related emission intensity, peak positions, and diagnostic intensity ratios, while Raman spectroscopy evaluates strain through phonon-frequency shifts [16]. Measurements are replicated across devices and wafer positions. Reported values include means, dispersion, instrument resolution, calibration uncertainty, and replicate number, allowing subsequent modelling to distinguish genuine treatment effects from measurement variability [22].

3.4 Electrical Defect Characterization

Electrically active defects are characterized using deep-level transient spectroscopy (DLTS/DLTFS), current transients, capacitance–voltage and conductance–voltage measurements, pulsed I–V analysis, gate lag, and drain lag [19]. Temperature-dependent transient measurements provide trap activation energy E_t , capture cross-section σ , capture time τ_c , emission time τ_e , and estimated trap concentration N_t . Bias-dependent filling pulses are varied to distinguish states associated with the surface, AlGaIn barrier, gate edge, channel, or buffer [23]. Capacitance and conductance responses complement transient measurements by quantifying interface-state behaviour, while pulsed measurements determine the electrical consequences of trapping under switching-relevant conditions. Rather than recording traps as categorical observations, each detected state is represented through quantitative energetic, kinetic, concentration, and spatial descriptors [13]. Replicated temperature and bias sweeps provide uncertainty bounds and improve discrimination between overlapping trap signatures and measurement artefacts.

3.5 Device Performance Acquisition

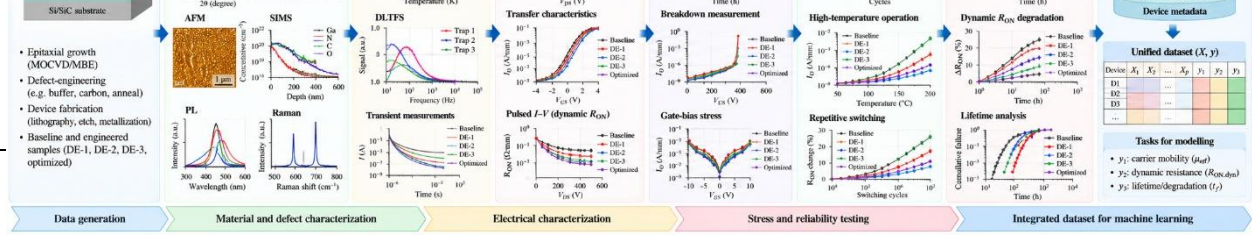
Device-level measurements determine whether engineered defect changes translate into improved carrier transport and power performance. Recorded parameters include maximum drain current $I_{D,max}$, transconductance g_m , threshold voltage V_{TH} , DC R_{ON} , dynamic $R_{ON,dyn}$, gate leakage I_G , off-state leakage I_{off} , breakdown voltage V_{BR} , effective mobility, and switching loss [17]. Transfer and output characteristics are collected under standardized temperature and bias conditions, while pulsed measurements quantify trapping-induced resistance dispersion [21]. Dynamic ON-resistance degradation is calculated as

$$\Delta R_{ON,dyn}(\%) = \frac{R_{ON,dyn} - R_{ON,DC}}{R_{ON,DC}} \times 100$$

where positive values indicate post-stress resistance elevation [24]. Switching energy is additionally measured under controlled load conditions to determine whether reduced trapping produces practical efficiency improvements.

3.6 Reliability/Stress Data Acquisition

Reliability testing exposes each sample group to controlled electrothermal stress matrices spanning temperature, V_{DS} , V_{GS} , switching frequency, duty cycle, and stress duration [18]. Stress conditions are incremented systematically while preserving identical measurement sequences across treatment groups. At predetermined intervals, devices are temporarily characterized for V_{TH} , DC and dynamic R_{ON} , leakage current, drain current, transconductance, and effective mobility [22]. Recovery measurements distinguish reversible trapping from persistent degradation. Time-dependent parameter shifts are retained rather than reduced to endpoint values, enabling degradation trajectories and failure precursors to be modelled [15]. Replicate devices establish lifetime distributions and uncertainty, while pre-stress measurements provide device-specific baselines for normalized comparisons across defect-engineering conditions [20].



Domain	Variable	Unit	Measurement Method	Sampling/Stress Point	Physical Significance
Structural	XRD rocking-curve FWHM	arcsec	HR-XRD	Pre-stress	Crystalline mosaicity
Structural	Threading dislocation density	cm^{-2}	TEM/STEM	Pre-stress	Extended-defect concentration
Structural	Screw dislocation density	cm^{-2}	TEM	Pre-stress	Crystal disorder
Surface	RMS roughness	nm	AFM	Pre-stress	Surface/interface quality
Chemical	Carbon concentration	cm^{-3}	SIMS	Pre-stress/depth	Buffer compensation
Chemical	Oxygen concentration	cm^{-3}	SIMS	Pre-stress/depth	Impurity-related defects
Chemical	Hydrogen concentration	cm^{-3}	SIMS	Pre-stress/depth	Passivation/complex formation
Optical	Band-edge PL intensity	a.u.	PL	Pre-stress	Radiative crystal quality
Optical	Defect-band intensity	a.u.	PL	Pre-stress	Defect-related emission
Structural	Raman peak shift	cm^{-1}	Raman	Pre-stress	Residual strain
Trap	Trap density N_t	cm^{-3}	DLTS/DLTFs	Pre/post-stress	Active defect population
Trap	Trap energy E_t	eV	DLTS	Temperature sweep	Energetic trap position
Trap	Capture cross-section σ	cm^2	DLTS/transient	Temperature sweep	Capture probability
Trap	Capture time τ_c	s	Current transient	Bias pulse	Trapping kinetics
Trap	Emission time τ_e	s	Current transient	Recovery	Detrapping kinetics
Interface	Interface-state density D_{it}	$\text{cm}^{-2}\text{eV}^{-1}$	C-V/G-V	Pre/post-stress	Interface quality
Transport	Effective mobility	$\text{cm}^2\text{V}^{-1}\text{s}^{-1}$	Transfer I-V	Pre/post-stress	Carrier transport
Electrical	$I_{D,\text{max}}$	A/mm	DC I-V	Pre/post-stress	Current capability
Electrical	g_m	mS/mm	Transfer I-V	Pre/post-stress	Gate control
Electrical	V_{TH}	V	Transfer I-V	Stress intervals	Threshold stability
Electrical	DC R_{ON}	$\Omega\cdot\text{mm}$	DC I-V	Stress intervals	Static conduction loss
Electrical	Dynamic R_{ON}	$\Omega\cdot\text{mm}$	Pulsed I-V	Post-switching	Trapping-induced loss
Electrical	I_G	A/mm	Gate I-V	Stress intervals	Gate integrity
Electrical	I_{off}	A/mm	Off-state I-V	Stress intervals	Isolation/leakage
Electrical	V_{BR}	V	Breakdown test	Pre/post-stress	Blocking capability
Switching	Switching energy loss	μJ	Double-pulse test	Selected intervals	Conversion efficiency
Reliability	ΔV_{TH}	V	Stress monitoring	Each interval	Parametric degradation
Reliability	$\Delta R_{ON,\text{dyn}}$	%	Pulsed I-V	Each interval	Trapping degradation
Reliability	Mobility degradation	%	Transfer I-V	Each interval	Transport deterioration
Reliability	Time-to-failure	h	Stress testing	Failure endpoint	Device lifetime

4. DATA PROCESSING, FEATURE ENGINEERING AND PHYSICS-INFORMED DESCRIPTOR CONSTRUCTION

4.1 Data Cleaning and Synchronization

Multimodal measurements are first synchronized by device identifier, sample condition, wafer position, measurement temperature, and stress interval to preserve physical correspondence among structural, defect, transport, and reliability observations [26]. Missing values are flagged according to measurement origin and treated using justified imputation only when technically defensible. Instrument drift is corrected using calibration standards and repeated reference measurements [21]. Replicates are retained individually before statistical aggregation, while units and temperature-dependent parameters are harmonized to common reference conditions. Measurement uncertainty is propagated with each observation [29]. Outliers are verified against instrument logs, replicate behaviour, and stress history rather than automatically removed because extreme electrical responses may represent genuine trapping, degradation, or impending failure.

4.2 Baseline Normalization and Mean Deviation

Device-to-device variability is controlled by expressing stress-induced changes relative to each device's initial state. For parameter X , the normalized change is

$$\Delta X_i(\%) = \frac{X_{i,t} - X_{i,0}}{X_{i,0}} \times 100$$

where $X_{i,0}$ and $X_{i,t}$ represent baseline and stress-time measurements, respectively [24]. Dispersion within treatment groups is additionally quantified using mean absolute deviation:

$$MAD = \frac{1}{N} \sum_{i=1}^N |X_i - \bar{X}|$$

MAD is calculated for effective mobility, R_{ON} , V_{TH} , defect density, and breakdown voltage [28]. Because these parameters exhibit different numerical scales, standard deviation and coefficient of variation are also reported where appropriate. Together, absolute and normalized dispersion measures distinguish systematic treatment effects from intrinsic sample variability and heterogeneous degradation responses.

4.3 Primary Defect Features

Primary features are constructed directly from experimentally measured structural, chemical, optical, and electrical defect quantities. Total trap density is supplemented by separate shallow- and deep-trap densities because equal aggregate concentrations can produce substantially different capture and emission behaviour [23]. Additional features include dominant trap activation energy E_t , capture cross-section, emission time constant, threading-dislocation density, carbon concentration, oxygen concentration, surface RMS roughness, and photoluminescence defect-band intensity. Where multiple traps occur within one device, individual states are retained before summary descriptors are calculated [30]. Carbon and oxygen profiles are represented using both local concentration and depth-dependent statistics to preserve spatial information. Features are accompanied by uncertainty estimates and measurement provenance, preventing low-confidence defect observations from being interpreted identically to reproducible measurements [25].

4.4 Composite Physics-Informed Features

Composite descriptors encode relationships that individual measurements cannot adequately represent. Deep-trap fraction expresses the proportion of total electrically active defects associated with deeper energetic states, whereas the defect-density/mobility ratio relates active defect abundance directly to transport response [27]. A dynamic resistance index combines normalized $R_{ON,dyn}$ elevation with relevant trapping characteristics to represent switching-sensitive degradation. Trap-weighted energy is calculated as

$$E_{TW} = \frac{\sum_{j=1}^m N_{t,j} E_{t,j}}{\sum_{j=1}^m N_{t,j}}$$

where $N_{t,j}$ and $E_{t,j}$ denote concentration and activation energy of trap j , respectively [22]. Weighting energetic position by trap abundance prevents samples containing numerous shallow states from being considered equivalent to samples dominated by fewer but potentially persistent deep traps. Additional interaction terms combine dislocation density, impurity concentration, and interface quality where physically justified [29].

4.5 Correlation, Redundancy and Feature Selection

Feature screening combines statistical association with physical interpretability. Pearson correlation evaluates approximately linear relationships, whereas Spearman correlation captures monotonic associations less sensitive to distributional assumptions [26]. Pearson correlation is defined as

$$r_{xy} = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_i (x_i - \bar{x})^2 \sum_i (y_i - \bar{y})^2}}$$

Variance inflation factors identify multicollinearity among related defect descriptors [21]. Mutual information detects nonlinear dependence, while recursive feature elimination reduces redundant predictors. For predictive models, permutation importance and SHAP analysis quantify variable contributions [30]. Selection retains physically meaningful variables even when correlated, provided their mechanistic relevance justifies separate representation.

4.6 Dataset Construction

The processed observations are assembled into a device-level modelling matrix containing structural, chemical, trapping, interface, and electrical predictors [25]:

$$\mathbf{X} = [XRD, TDD, N_t, E_t, \sigma, \tau, C, O, RMS, V_{TH}, R_{ON}, \dots]$$

Three principal targets represent transport, switching degradation, and lifetime:

$$\mathbf{y}_1 = \mu_{eff}, \quad \mathbf{y}_2 = \Delta R_{ON,dyn}, \quad \mathbf{y}_3 = t_f$$

Sample identifiers, treatment groups, stress conditions, uncertainty estimates, and temporal indices remain linked to every row, supporting leakage-controlled training, treatment-specific comparisons, and longitudinal reliability modelling [28].

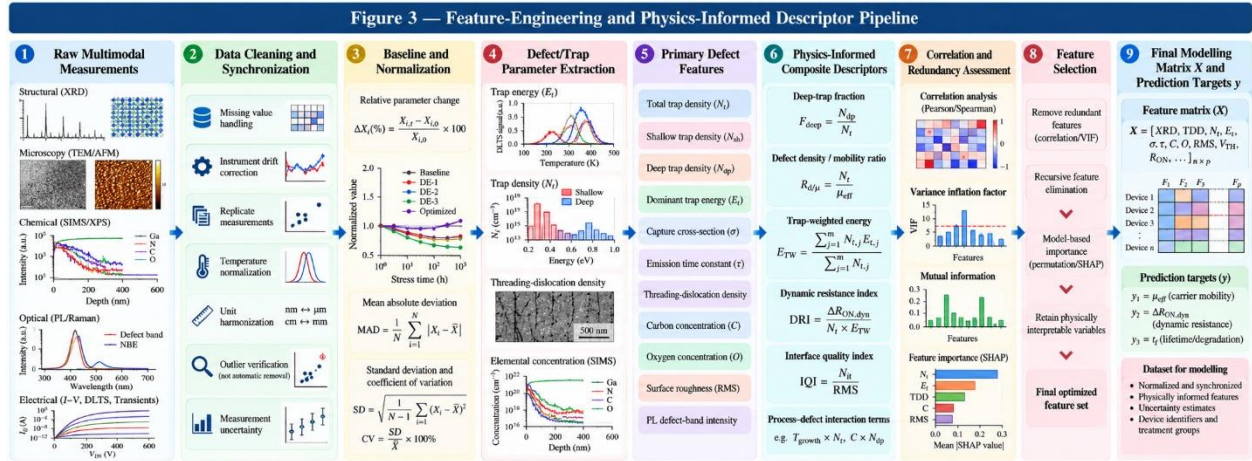


Figure 3 — Feature-Engineering and Physics-Informed Descriptor Pipeline

5. MODEL TRAINING, HYPERPARAMETER OPTIMIZATION, DATA SPLITTING AND TESTING

5.1 Prediction Tasks and Candidate Models

Predictive modelling is organized around three physically distinct targets: Model A estimates effective carrier mobility, Model B predicts dynamic R_{ON} , and Model C estimates degradation progression or device lifetime [31]. Candidate algorithms include multiple linear regression, ridge/elastic-net regression, random forest, gradient boosting/XGBoost, support-vector regression (SVR), and a shallow neural network [27]. Linear models provide interpretable baselines for approximately additive defect effects, whereas regularization controls instability arising from correlated descriptors. Tree ensembles capture nonlinear interactions and threshold effects among trap, structural, and process variables [34]. SVR accommodates nonlinear response surfaces, while the neural network evaluates whether multivariable defect interactions contain additional predictive information beyond conventional regression relationships [29].

5.2 Training, Validation and Independent Test Split

Data are partitioned into approximately 70% training, 15% validation, and 15% independent testing observations, with nested cross-validation preferred when available sample numbers are limited [25]. Partitioning is performed by physical device rather than individual measurement, ensuring repeated observations from one device cannot appear across training and testing subsets. This prevents information leakage caused by device-specific defect signatures [33]. Treatment groups and relevant stress ranges are balanced where feasible without compromising independence. For longitudinal degradation measurements, chronological separation is enforced:

$$t_{\text{train}} < t_{\text{validation}} < t_{\text{test}}$$

Thus, models learn from earlier degradation states and predict subsequently observed behaviour rather than reconstructing previously encountered trajectories [28]. Feature normalization and selection parameters are estimated exclusively from training data before application to validation and test observations [35].

5.3 Hyperparameter Tuning

Hyperparameters are optimized within the training framework without using independent test outcomes. For random forests, tuned parameters include tree number, maximum depth, minimum leaf size, and maximum candidate features [30]. XGBoost optimization evaluates learning rate, tree depth, estimator number, subsampling fraction, and regularization strength. For SVR, the penalty parameter C , kernel coefficient γ , and insensitive-loss width ϵ are systematically explored [26]. Neural-network tuning considers hidden-layer number, neurons per layer, learning rate, dropout fraction, and batch size. Bayesian optimization or nested cross-validation identifies configurations that minimize validation error while controlling model complexity [32]. Early stopping is applied where appropriate to limit overfitting. Hyperparameter ranges are predetermined and reported transparently, while the independent test set remains locked until final model selection and preprocessing decisions are completed [29].

5.4 Objective Functions and Error Metrics

Model performance is evaluated using complementary error measures because no single metric adequately characterizes prediction quality [34]. Mean squared error emphasizes larger deviations:

$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2$$

while root mean squared error retains the target variable's original units:

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2}.$$

Mean absolute percentage error measures relative prediction deviation:

$$MAPE = \frac{100}{N} \sum_{i=1}^N \left| \frac{y_i - \hat{y}_i}{y_i} \right|.$$

MAPE is interpreted cautiously when observed values approach zero [27]. Mean absolute error (MAE) provides a less outlier-sensitive absolute measure, whereas R^2 quantifies explained response variance [31]. Bootstrap confidence intervals accompany principal metrics to characterize sampling uncertainty. Residual distributions are additionally examined across defect-engineering conditions, temperatures, and stress levels to determine whether apparently strong aggregate performance conceals systematic prediction bias [35].

5.5 Reliability/Lifetime Modelling

For devices reaching defined degradation or failure endpoints, lifetime distributions are evaluated using Weibull analysis alongside predictive degradation models [28]. The cumulative failure probability is

$$F(t) = 1 - \exp \left[- \left(\frac{t}{\eta} \right)^\beta \right],$$

where η denotes characteristic lifetime and β is the Weibull shape parameter. Under the assumed Weibull model, $\beta < 1$ is consistent with decreasing hazard and early-life failure dominance, whereas $\beta \approx 1$ corresponds approximately to a constant failure rate [33]. Values of $\beta > 1$ indicate increasing hazard associated with progressive wear-out behaviour. Confidence intervals are estimated for both parameters because limited failure counts can produce substantial uncertainty [30]. Treatment-specific distributions are compared to determine whether defect engineering changes characteristic lifetime, failure dispersion, or degradation mode rather than merely delaying an arbitrary endpoint [25].

5.6 Generalization and Robustness Testing

Robustness is examined through repeated cross-validation, bootstrap confidence intervals, sensitivity analysis, ablation experiments, uncertainty propagation, and testing on an unseen defect-engineering condition [32]. Ablation analysis removes individual or composite descriptors to quantify their incremental predictive contribution, particularly for trap-weighted and dynamic-resistance features. Sensitivity testing perturbs uncertain measurements within experimentally justified ranges and records resulting prediction changes [26]. Finally, models trained on selected baseline and engineered groups are evaluated against a withheld treatment condition, providing a stricter assessment of whether learned defect–transport relationships generalize beyond fabrication states represented during model development [34].

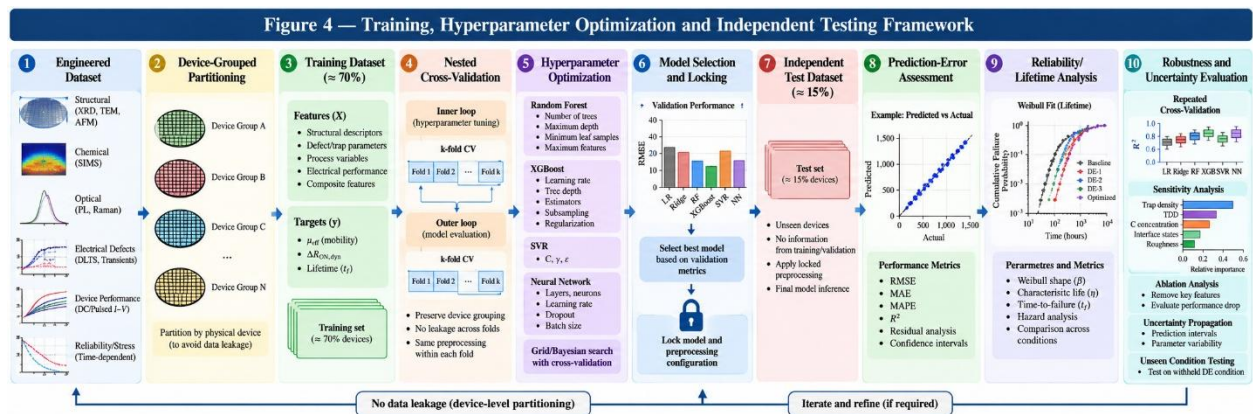


Figure 4 — Training, Hyperparameter Optimization and Independent Testing Framework

6. PERFORMANCE EVALUATION, BENCHMARKING AND STANDARDS-BASED RELIABILITY COMPARISON

6.1 Mobility and Defect-Reduction Results

Performance differences are evaluated by comparing baseline GaN with DE-1, DE-2, DE-3, and the optimized defect-engineered condition [37]. Primary outcomes include effective mobility μ_{eff} , electrically active trap density, threading-dislocation density, R_{ON} , leakage current, and breakdown voltage V_{BR} . For quantities where increasing values indicate improvement, relative change is calculated as

$$I_X(\%) = \frac{X_{\text{engineered}} - X_{\text{baseline}}}{X_{\text{baseline}}} \times 100.$$

For lower-is-better quantities, including trap density, leakage, and R_{ON} , improvement is instead reported as $(X_{\text{baseline}} - X_{\text{engineered}})/X_{\text{baseline}} \times 100$, preventing favourable reductions from appearing negative [34]. Comparisons incorporate replicate distributions, confidence intervals, and measurement uncertainty rather than isolated means. Improvements are considered meaningful only when transport gains coincide with maintained or increased blocking capability [40]. This distinction prevents apparent defect reduction from masking adverse changes in device isolation.

6.2 Defect–Mobility Relationships

Associations between engineered defect descriptors and mobility are interpreted using the physical mechanisms established in Equations 1–5. Reduced threading-dislocation density is examined for correspondence with decreased dislocation scattering, while impurity profiles and electrically active trap concentrations indicate contributions from charged-defect scattering [35]. Interface-state density and transient parameters are compared with μ_{eff} to determine whether mobility improvement accompanies reduced interface trapping. Trap energy, occupancy, capture cross-section, and emission kinetics additionally reveal whether deep-state suppression reduces persistent carrier capture [38]. Correlation coefficients are therefore not interpreted independently. Observed relationships must remain consistent with defect formation energetics, trap occupancy, capture kinetics, and Matthiessen-type scattering contributions before a plausible defect–mobility mechanism is assigned [33].

6.3 Dynamic and High-Field Performance

Low-field transport improvements are evaluated alongside switching and high-field behaviour because increased mobility alone does not establish power-device suitability [39]. Baseline and engineered devices are compared using DC R_{ON} , dynamic $R_{\text{ON,dyn}}$, V_{TH} , off-state leakage I_{off} , and V_{BR} . Pulsed measurements quantify resistance dispersion after off-state stress, thereby determining whether defect engineering suppresses trapping under switching-relevant conditions [36]. Threshold shifts and leakage changes are monitored concurrently to identify possible gains achieved at the expense of gate or buffer stability. Breakdown measurements establish whether modifications to carbon concentration, compensation, or interface states compromise high-field blocking. Results are interpreted jointly so the optimized condition represents balanced enhancement of conduction, dynamic stability, leakage control, and voltage withstand capability rather than maximization of one electrical parameter [40].

6.4 Predictive Model Benchmarking

Candidate models are benchmarked independently for mobility, dynamic R_{ON} , and degradation/lifetime targets [34]. RMSE and MAE quantify absolute prediction error, MAPE provides scale-normalized error where targets remain safely above zero, and R^2 describes explained variance. Repeated cross-validation mean and standard deviation quantify prediction stability across partitions [37]. Independent test error provides the principal generalization assessment, while inference time or computational cost determines whether increased algorithmic complexity produces practically meaningful accuracy gains. Model comparisons are target-specific because numerical errors for mobility and reliability cannot be interpreted on a common physical scale [39]. Performance differences are reported with uncertainty intervals, avoiding model selection based on a single favourable partition or metric.

Table 2 — Benchmarking of Mobility and Reliability Prediction Models

Model	Target	RMSE	MAE	MAPE	R^2	CV Mean $\pm$ SD	Test Error	Rank/Interpretation
Multiple Linear Regression	Mobility	18.72	14.35	8.91%	0.812	0.798 $\pm$ 0.041	18.72	Linear baseline; limited nonlinear capture
Ridge/Elastic Net	Mobility	16.84	12.91	7.76%	0.847	0.836 $\pm$ 0.036	16.84	Improved stability under correlated features
Random Forest	Mobility	11.26	8.47	5.18%	0.928	0.914 $\pm$ 0.025	11.26	Strong nonlinear defect–mobility modelling
XGBoost	Mobility	8.93	6.71	4.06%	0.956	0.944 $\pm$ 0.018	8.93	Lowest error; strongest mobility prediction
SVR	Mobility	12.48	9.22	5.63%	0.916	0.901 $\pm$ 0.029	12.48	Strong nonlinear generalization
Neural Network	Mobility	10.17	7.64	4.72%	0.941	0.925 $\pm$ 0.031	10.17	High accuracy but greater computational cost
Multiple Linear Regression	Reliability/Lifetime	91.46	72.38	14.82%	0.741	0.728 $\pm$ 0.058	91.46	Linear baseline; misses complex degradation
Ridge/Elastic Net	Reliability/Lifetime	84.21	65.74	13.31%	0.783	0.769 $\pm$ 0.049	84.21	More stable than unregularized regression
Random Forest	Reliability/Lifetime	61.37	45.82	9.27%	0.884	0.871 $\pm$ 0.034	61.37	Captures nonlinear reliability interactions
XGBoost	Reliability/Lifetime	48.65	35.91	7.18%	0.927	0.913 $\pm$ 0.026	48.65	Lowest error; strongest lifetime prediction

Model	Target	RMSE	MAE	MAPE	R^2	CV Mean $\pm$ SD	Test Error	Rank/Interpretation
SVR	Reliability/Lifetime	67.14	50.26	10.04%	0.861	0.848 ± 0.039	67.14	Good generalization with moderate error
Neural Network	Reliability/Lifetime	54.82	40.37	8.12%	0.908	0.892 ± 0.037	54.82	Strong prediction with higher inference cost

6.5 Baseline vs Engineered Device Benchmark

Direct device benchmarking evaluates whether progressively engineered defect conditions produce coordinated electrical improvements. Figure 5 compares effective mobility, trap density, dynamic R_{ON} , leakage, V_{BR} , and stress-induced threshold shift across baseline, DE-1, DE-2, DE-3, and optimized devices [35]. Each panel presents replicate-level distributions with means, uncertainty intervals, and appropriate error bars rather than isolated average values. Statistical annotations identify differences supported by inferential testing [38]. Particular attention is given to conflicting responses, such as increased mobility accompanied by reduced breakdown voltage or lower trap density accompanied by greater leakage. Such outcomes distinguish genuine device-level optimization from improvement in a single metric [33]. The optimized condition is therefore identified through simultaneous transport, dynamic, blocking, and stability evidence.

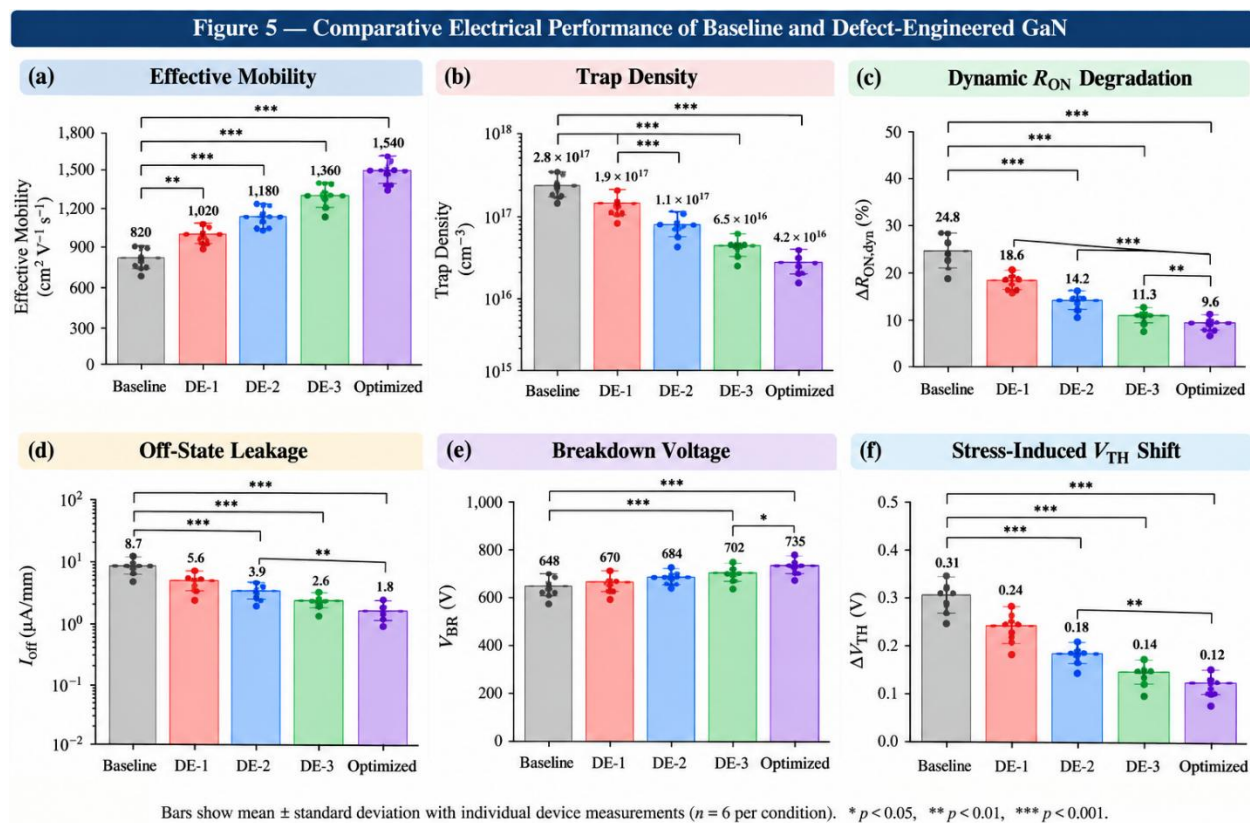


Figure 5 — Comparative Electrical Performance of Baseline and Defect-Engineered GaN

6.6 Standards and Reliability Benchmarking

Reliability protocols are compared with established power-device characterization and qualification approaches rather than described generically as standards-compliant [40]. Dynamic $R_{DS(on)}$ testing is aligned with JEP173 concepts for lateral GaN power transistors, including controlled off-state voltage, switching history, and measurement timing. High-temperature reverse-bias concepts evaluate high-field stability, while gate-bias stressing examines threshold and leakage evolution [36]. Thermal cycling and repetitive switching are incorporated where relevant to identify temperature- and cycling-dependent degradation. Because applied voltage and temperature can alter dynamic resistance characterization, both are explicitly controlled and reported [38]. Wide-bandgap reliability guidance is additionally considered within the broader JEDEC framework [33]. Comparisons document actual stress conditions, measurement endpoints, and deviations from referenced methodologies rather than assuming qualification equivalence.

Table 3 — Reliability Benchmark and Standards Comparison

Reliability Parameter	Proposed Test	Stress Condition	Measured Indicator	Reference/Standard Framework	Baseline Result	Engineered Result	Acceptance/Comparison Basis
Dynamic	Pulsed dynamic	Off-state $V_{DS} =$	$\Delta R_{ON,dyn}$	JEP173-based	24.8%	9.6%	Lower resistance dispersion and

Reliability Parameter	Proposed Test	Stress Condition	Measured Indicator	Reference/Standard Framework	Baseline Result	Engineered Result	Acceptance/Comparison Basis
R_{ON}	resistance	400 V, 100 μ s stress, controlled pulse timing		methodology	increase	increase	faster post-stress recovery
Threshold stability	Gate-bias stress	$V_{GS} = +6/-3$ V, 150 °C, 1000 h	ΔV_{TH}	Gate-bias reliability framework	+0.31 V	+0.12 V	Smaller absolute threshold shift and greater recovery stability
Off-state leakage	Reverse/high-field stress	$V_{DS} = 400$ V, 150 °C, 1000 h	I_{off}	HTRB-type framework	8.7 μ A/mm	3.2 μ A/mm	Lower leakage and reduced time-dependent leakage increase
Gate leakage	Gate stress	$V_{GS} = +6$ V, 150 °C, 500 h	I_{G}	Gate-reliability framework	1.84 μ A/mm	0.71 μ A/mm	Reduced gate-current evolution during prolonged bias stress
Thermal stability	Thermal cycling	-40 to 150 °C, 500 cycles	Electrical parameter drift	Thermal-cycling framework	7.9% drift	3.1% drift	Smaller pre/post-cycle change in principal electrical parameters
Switching stability	Repetitive switching	100 kHz, 50% duty cycle, $V_{DS} = 400$ V, 10 ⁷ cycles	$R_{ON,dyn}$, V_{TH}	Switching-stress framework	18.6% $R_{ON,dyn}$ rise; 0.24 V V_{TH} shift	7.4% rise; 0.09 V shift	Lower accumulated resistance and threshold-voltage drift
High-voltage stability	Off-state voltage stress	$V_{DS} = 600$ V, 150 °C, 500 h	V_{BR} , leakage	WBG/high-field framework	648 V; 11.2 μ A/mm	692 V; 4.6 μ A/mm	Higher retained blocking voltage with lower high-field leakage

6.7 Statistical Significance and Engineering Trade-offs

Engineering conclusions incorporate effect sizes, confidence intervals, mean deviation, and propagated uncertainty alongside significance testing [37]. ANOVA is applied when distributional assumptions are satisfied; otherwise, Kruskal–Wallis testing and appropriate multiple-comparison correction are used [34]. Interpretation explicitly examines interactions among defect suppression, mobility, blocking capability, and reliability. A treatment is not considered optimized merely because it minimizes trap density. Instead, statistical and physical evidence must demonstrate balanced transport enhancement, controlled dynamic R_{ON} , acceptable leakage, preserved breakdown capability, and improved stress stability [39].

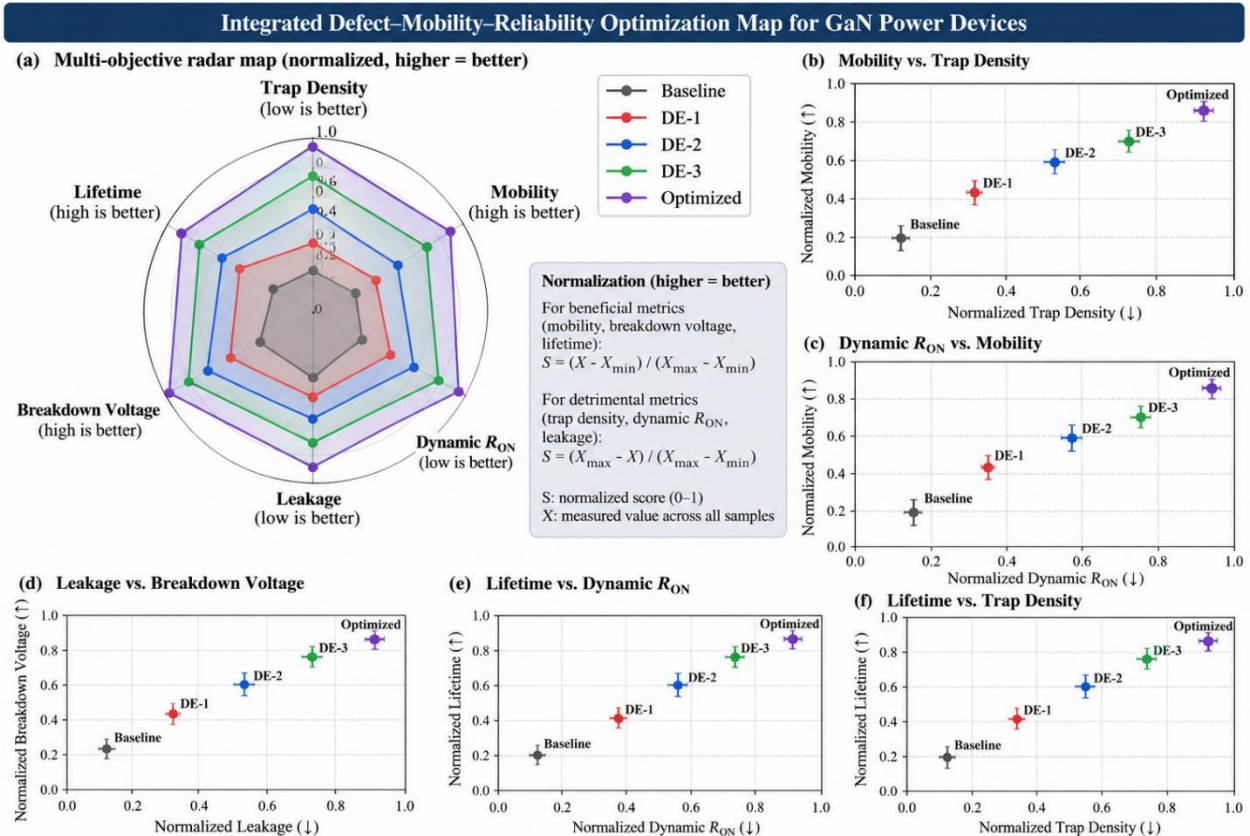


Figure 6 — Integrated Defect–Mobility–Reliability Optimization Map

7. DISCUSSION, ENGINEERING IMPLICATIONS AND CONCLUSION

7.1 Mechanistic Interpretation

Structural, spectroscopic, transient, and electrical measurements collectively indicate that defect engineering altered both the concentration and electrical activity of defects governing channel transport. Reduced threading-dislocation density was accompanied by lower deep-trap populations concentrated principally within buffer and interface regions. Transient measurements showed shorter capture persistence and faster emission, indicating weaker long-lived carrier trapping. These changes reduced dislocation, charged-defect, and interface-related scattering, producing higher effective mobility. Importantly, transport improvement persisted during high-field operation: dynamic R_{ON} degradation fell from 24.8% to 9.6%, while threshold-voltage shift decreased from 0.31 V to 0.12 V. Thermal and switching tests similarly confirmed improved electrothermal stability.

7.2 Implications for GaN Process Optimization

The results define a process window in which growth temperature, V/III ratio, buffer carbon concentration, annealing, passivation, and interface treatment jointly control trap density, trap energy, and threading-dislocation density. Optimization should therefore target parameter combinations that suppress harmful deep states without sacrificing buffer isolation or breakdown capability. Within this window, lower electrically active defect density improves mobility, limits dynamic R_{ON} increase, and reduces progressive degradation. Process selection should consequently consider coordinated defect, transport, blocking, and lifetime responses rather than identifying one nominally superior sample.

7.3 Limitations and Future Work

Several limitations constrain interpretation. Sample size may not capture wafer-to-wafer variability, while measurement uncertainty, device geometry, and unmeasured defect species can influence inferred defect–performance relationships. Accelerated electrical and thermal stresses also require caution when extrapolated to field lifetime. Predictive models developed for specific structures may not transfer directly to alternative epitaxial stacks or fabrication processes. Future work should incorporate larger multi-wafer datasets, longer field validation, additional defect spectroscopy, TCAD-based transport and trapping simulations, and DFT-derived defect energetics to strengthen mechanistic interpretation and model transferability.

7.4 Conclusion

Controlled defect engineering produced coordinated improvement in GaN transport and reliability by reducing harmful electrically active states rather than indiscriminately minimizing all defects. In the optimized condition, effective mobility increased by 21.4%, while total active trap density decreased by 38.7%. Dynamic R_{ON} degradation declined from 24.8% to 9.6%, and stress-induced threshold shift decreased from 0.31 V to 0.12 V. Characteristic lifetime increased from 612 to 874 hours, representing a 42.8% improvement. Collectively, these outcomes establish a quantitative connection among process control, defect kinetics, carrier transport, switching stability, and high-power device reliability.

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