

Metastable defects in III-nitrides (Review)

A.E. Belyaev

V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, Kyiv, Ukraine

E-mail: belyaev@isp.kiev.ua

Abstract. Metastable states in III-nitrides (AlN, GaN, InN and their alloys) are an important topic in materials science, device physics, and epitaxial growth because these compounds exhibit multiple competing crystal structures, defect configurations, and phase behavior that strongly affect optical, electrical, and mechanical properties. The paper is a concise, structured review-style summary covering the main concepts, mechanisms, experimental signatures, theoretical approaches, and device implications. Actions that should be proposed to avoid the effects of metastable defects in III-nitride based devices are discussed. Avoiding metastable defect effects in III-nitride devices requires preventing their formation (through growth and doping control), stabilizing their electronic configuration (by annealing or optical activation), and designing device architectures that minimize field- or temperature-induced transitions. These combined actions ensure consistent carrier density, higher mobility, and superior optical and electrical reliability in GaN-, AlGaIn-, and InGaIn-based devices.

Keywords: metastable defects, III-nitrides, electronic configuration, field- or temperature-induced transitions.

<https://doi.org/10.15407/spqeo29.03.283>

PACS 61.72.Bb, 61.72.J-, 71.55.Eq

Manuscript received 11.07.26; revised version received 26.08.26; accepted for publication 16.09.26; published online 25.09.26.

Intrinsic and extrinsic metastable centers

Metastable defects in III-nitrides (GaN, AlGaIn and GaN/AlGaIn heterostructures) are defect states that can exist in more than one stable configuration, often depending on factors such as temperature, illumination, or charge state. These defects significantly influence the optical and electronic behavior of III-nitrides, which is crucial for electronic and optoelectronic devices such as high-electron-mobility transistors (HEMTs), light-emitting diodes (LEDs), and laser diodes (LDs) [1]. Research has identified both intrinsic (native) and extrinsic (impurity-related) metastable centers [2]. First, let's consider gallium nitride's possibilities for forming metastable states. Native defects such as gallium and nitrogen vacancies are among the most studied [3, 4]. Nitrogen vacancies (V_N) can act as shallow donors, while Ga vacancies (V_{Ga}) act as deep acceptors. Both can form metastable complexes under different charge states. Recent DFT and hybrid-functional calculations show that V_N can exhibit negative-U behavior, meaning one charge state (e.g., $2+$) is unstable, and transitions skip it – a hallmark of metastability [5]. Experimentally, metastable defects associated with V_{Ga} were found to produce blue and yellow luminescence bands, which switch intensity depending on temperature and excitation. These centers

may trap holes and show luminescence fatigue – they lose intensity under continuous illumination but recover at room temperature.

Expanding the functionality of III-nitride-based devices requires the use of intentional doping. However, impurity-related metastable defects may form in this case. For example, Eu-doped gallium nitride (GaN) is a promising candidate for GaN-based red light-emitting diodes, which are needed for future micro-display technologies. Introducing a superlattice structure comprised of alternating undoped and Eu-doped GaN layers has been observed to lead to an order-of-magnitude increase in output power [6]. Europium (Eu^{3+}) introduces metastable defect complexes, specifically ($Eu_{Ga}-V_N$). *Ab initio* calculations reveal two stable configurations – axial and basal – each with distinct energies and electronic levels. These states can switch depending on the charge state of the defect, producing charge-state controlled metastability [7, 8].

Magnesium (Mg) is the most used *p*-type dopant for GaN [9, 10]. Mg-related metastable behavior is observed in near-bandgap UV luminescence, where the luminescence spectrum evolves under electron irradiation. The process is reversible with heat, attributed to stacking-fault-related defect activation – suggesting metastability stems from irradiation-induced defect rearrangement [11].

It should be noted how the above-mentioned defects manifest themselves. First, several broad photoluminescence (PL) bands (e.g., yellow, blue, green) in GaN are linked to metastable defect transitions. Second, metastability leads to temperature- and light-dependent emission switching, persistent photoconductivity, and luminescence fatigue effects. As a result, understanding these centers is crucial for controlling nonradiative recombination and improving GaN-based devices' efficiency. In essence, metastable defects in GaN arise from both intrinsic vacancies and impurity-defect complexes (like Eu- or Mg-related). They exhibit charge-state or configuration-dependent bistability that affects optical emissions and carrier dynamics – making their characterization vital for high-performance photonic and electronic applications.

Recently, a lot of attention has been paid to impurities, which, along with hydrogen-like states, can form states with negative correlation energy, the so-called DX states. DX centres were first identified in AlGaAs alloys, and the very detailed studies of donors in these alloys are the most relevant benchmarks for the characterisation and the theoretical models used to understand DX behavior in other materials [12].

In the AlGaN alloy system, three initial investigations of the DX behavior of donors have been published [13–15].

Silicon (Si) on Ga sites (Si_{Ga}) is the most studied DX-forming dopant in GaN. In pure GaN at ambient pressure, silicon typically acts as a shallow donor (responsible for n -type conductivity). Under high pressure, high Al content in $\text{Al}_x\text{Ga}_{1-x}\text{N}$, or compensating conditions, Si_{Ga} can undergo a DX transition, producing a deep, metastable configuration with strong localization of one electron and lattice distortion. Negative-U behavior is observed in Al-rich alloys – the DX center becomes more favorable as Al content increases beyond $x \approx 0.4 - 0.5$ in AlGaN [16]. Si is an established shallow n -type dopant in GaN and $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ($x < 0.8$). However, an increased ionization energy is observed for Si in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ (for $x > 0.8$) that is commonly attributed to the formation of a DX center, consequently limiting the achievable conductivity in high-Al-content AlGaN [17–20].

Germanium (Ge) acts as a shallow donor in GaN and is sometimes used as an alternative to Si. Under high pressure or in Al-rich environments, Ge-induced DX formation has been predicted theoretically, but experimentally, Ge remains largely stable and shallow in GaN. The DX configuration becomes more relevant in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys for $x > 0.5$, similar to Si. The behavior of the Ge dopant in AlGaN was studied as a function of Al content in the alloy. At Al compositions below 40%, it behaved as a shallow donor with ionization energy below 20 meV. At Al compositions above 40%, it emerged as a deep donor, whose ionization energy increased with increasing Al content and reached 150 meV for AlGaN with 60% Al. At this point, only the deep donor state was observed [21].

Oxygen is a common unintentional donor in GaN. First-principles studies predict that O_{N} can form DX-like centers at high Al concentration in AlGaN alloys [22, 23].

In GaN itself, O_{N} is generally shallow, but in AlGaN with Al $> \sim 30\text{--}40\%$, it may behave as a deep DX-like donor due to conduction-band lowering and local relaxation effects.

Heavy donors, such as Te and Se, have been suggested (by first-principles studies) to induce deeper DX-like configurations even in GaN, but experimental verification is scarce [24, 25]. These dopants are rarely used due to incorporation challenges and amphoteric behavior.

As a result, in pure GaN, classic DX centers are rare – most donors (Si, O, Ge) remain shallow.

However, as the local environment changes (pressure, Al incorporation, strain, or high electric field), these donors can transform into metastable, deep DX-like states, strongly affecting carrier compensation and device reliability. In Table I, DX center formation trends are summarized.

In aluminum nitride (AlN), DX centers are theoretically and experimentally predicted to be even more stable and deeper than in GaN because of AlN's wider bandgap (~ 6.2 eV), stronger ionicity, and larger lattice relaxation energy. The presence and behavior of DX centers in AlN are therefore crucial for understanding the electrical compensation and n -type doping limits in Al-rich alloys ($\text{Al}_x\text{Ga}_{1-x}\text{N}$). A DX center forms when a donor impurity undergoes a large lattice relaxation after capturing an electron, moving to an off-center position and creating a deep-level configuration. Because AlN is more ionic and has a deeper conduction band minimum (CBM) than GaN, donors that are shallow in GaN often become deep or unstable (DX-like) in AlN [26–30]. In Table II, likely DX-forming dopants are presented.

The DX configuration corresponds to a large displacement (~ 0.4 Å) of the donor atom toward a neighboring nitrogen atom, creating a broken bond and a localized electron. Negative-U behavior is common: the singly charged state (d^0) is unstable, and the defect transitions directly between d^+ and D^- due to lattice relaxation. Calculated capture barrier energies range from 0.2–1.0 eV, contributing to strong metastability and persistent photoconductivity effects. First-principles studies [22, 23] predict O_{N} and Si_{Al} donors that form deep DX levels in AlN with transition levels 1–2 eV below the conduction band. The manifestation of DX centers is observed in optical and electrical measurements (AlN doped with Si or O shows very low free-electron concentrations despite high impurity levels, consistent with self-compensation by DX centers and electron trapping) as well as in photo- and thermally stimulated conductivity (at elevated temperatures or under illumination, partial ionization of DX centers increases conductivity, but equilibrium returns upon cooling or in the dark). The presence of DX centers significantly affects device physics. DX formation is the main reason AlN is extremely difficult to dope n -type – most donors become deep and inactive. The crossover from shallow to DX behavior with increasing Al content defines the “DX transition composition” (typically 40–60% Al). Deep DX states can act as non-radiative recombination centers and trap states, affecting UV LED efficiency and reliability.

Table I.

Dopant	Site	DX formation in GaN	DX formation in AlGaN	Notes
Si	Ga	Weak / under pressure	Strong ($x > 0.4$)	Most studied case
Ge	Ga	Minimal	Appears for high Al fractions	Alternative to Si
O	N	Weak / metastable	Strong ($x > 0.3$)	Unintentional donor
Te, Se	N	Theoretical only	Possible	Not widely verified

Table II.

Dopant	Site	Behavior in AlN	Notes
Silicon (Si)	Al site	Forms deep DX-like state	Shallow in GaN, but deepens in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ for $x > 0.4-0.5$; in pure AlN, typically deep (> 0.4 eV)
Germanium (Ge)	Al site	Deep donor / possible DX	Similar to Si, predicted to form an off-center configuration; limited activation experimentally
Oxygen (O)	N site	Strong DX former	O_N becomes deep ($\approx 1-2$ eV below CBM); explains self-compensation and limited n -type doping
Sulfur (S)	N site	Deep-level DX	Predicted <i>via</i> first-principles to form deep donor levels > 1 eV below CBM
Tellurium, selenium (Te, Se)	N site	Deep and unstable	Theoretical DX character; experimental realization is very poor

In summary: DX centers in AlN are deep, strongly bound donor configurations – primarily involving Si and O impurities – that dominate compensation processes and limit n -type conductivity. Their formation energy decreases with Al content, making AlN and high-Al AlGaN alloys intrinsically prone to DX-related metastability and deep-donor behavior.

Effect of DX centers on properties of 2DEG in AlGaN/GaN heterostructures

In AlGaN/GaN heterostructures, DX centers, mainly those associated with donor impurities such as Si or O in the AlGaN barrier, have a substantial impact on the two-dimensional electron gas (2DEG) that forms at the interface. These centers affect both the formation and the stability of the 2DEG by altering charge supply, local electrostatics, and trap dynamics. It is well established that 2DEG arises from:

- The polarization discontinuity (spontaneous and piezoelectric polarization) between AlGaN and GaN, creating a built-in electric field.
- Donor impurities (intentionally added or residual, *e.g.*, Si, O) in the AlGaN barrier, which act as charge reservoirs supplying electrons to the interface.

First of all, one should consider the mechanisms by which DX centers affect the 2DEG. Among them are:

a. Charge supply modulation

- Some dopants (especially Si and O) in the AlGaN barrier can exist in two states:
 - Shallow donor (d^0): provides electrons to the 2DEG.
 - Deep DX state: traps electrons, unavailable for conduction.

- When a large fraction of donors convert into the DX state, the effective donor density drops, lowering the sheet carrier density of the 2DEG.
- At low temperatures or under bias stress, these DX centers can remain negatively charged, pinning or depleting the 2DEG.

b. Metastability and dynamic trapping

- The conversion between shallow and deep states is thermally or optically activated:
 - Cooling can freeze donors in the DX configuration, reducing 2DEG density.
 - Illumination or heating releases trapped electrons, increasing it again.
- This leads to persistent photoconductivity (PPC) or bias-stress hysteresis, revealing the metastable nature of DX centers.

c. Electric-field interaction

- The large polarization field in the AlGaN barrier ($\sim 1-2$ MV/cm) favors DX formation because it enhances local lattice relaxation around donors.
- During high-bias operation, field-induced electron emission from DX centers can cause threshold shifts or transient current increases.

d. Scattering and mobility degradation

- Ionized or neutral DX centers act as Coulombic scattering sites, reducing mobility, especially when their distribution is near the 2DEG channel.
- They also contribute to current collapse and dispersion in high-frequency devices (*e.g.*, HEMTs) through trap-assisted charge modulation.

According to the available literature, it is possible to summarize the effects observed in AlGaN/GaN heterostructures (Table III).

Table III.

Property	Typical observation	DX-related interpretation
2DEG density vs temperature	Decreases at low T , recovers after illumination	Electrons trapped in DX^- states
Persistent photoconductivity	Long-lived conductivity after UV or blue light	Photoionization of DX centers
Current collapse / gate lag	Transient current reduction after bias stress	Electron trapping in or near barrier DX centers
Hysteresis in $C-V$ or $I-V$ curves	Especially under slow sweep rates	Thermal recovery of metastable donors
Drain-induced barrier lowering artifacts	Time-dependent threshold drift	Field-assisted DX ionization

Based on this, we can make several recommendations to reduce the impact of metastable states, namely:

- Use of undoped or delta-doped barriers: reduces DX-related charge trapping.
- Lower Al content: below $\sim 40\%$, Si donors stay mostly shallow, minimizing DX formation.
- Thermal or optical activation: can intentionally reset or “de-trap” electrons from DX states.
- Alternative dopants (*e.g.*, Ge): shown to produce more stable, shallow donor behavior in mid-Al-content AlGaN.

In summary: DX centers in the AlGaN barrier act as metastable charge traps that dynamically control the electron transfer into the GaN channel. Their presence can lower carrier density, cause persistent photoconductivity or transient effects, and degrade mobility and reliability in AlGaN/GaN HEMT structures – especially in high-Al-content barriers where DX behavior is more pronounced.

The role of external factors

It is very important to consider the role of external factors, such as ultrasonic vibrations or microwave (including terahertz) radiation, on the effects associated with DX centers.

DX centers are strongly electron-phonon coupled systems; ultrasound effectively introduces a *coherent phonon population*. If the acoustic energy is comparable to a fraction of the DX barrier height (tens to hundreds of meV), it can significantly alter the equilibrium between the deep and shallow states, especially at moderate temperatures ($\sim 100 - 300$ K).

Ultrasonic vibrations can significantly influence DX centers in GaN and related III–V semiconductors by providing mechanical energy that couples to the local lattice strain and electronic configuration of the defect. The underlying mechanism is tied to how DX centers involve a strong electron-lattice relaxation – the donor atom moves off-center and distorts nearby bonds when it captures electrons. Ultrasonic waves introduce a periodic stress field that perturbs these local distortions.

Here’s how the effect works in more detail:

Strain coupling and potential-energy modulation

A DX center has two (or more) stable configurations:

- Shallow donor (d^0) – donor ion in its substitutional position, hydrogen-like shallow level.
- Deep DX^- state – donor atom displaced off-center, lattice distorted, deep localized level.

These two configurations are separated by an energy barrier on the configuration coordinate diagram. Ultrasonic strain modulates the local potential energy landscape. Acoustic pressure periodically alters the lattice spacing, changing bond angles and distances near the dopant (Si, O, *etc.*). This modulation can raise or lower the barrier between D^0 and DX^- states and even cause thermally assisted transitions between them. As a result, populations of shallow and deep states change dynamically – modifying the carrier concentration and conductivity.

Acoustically stimulated ionization and annealing

At suitable frequencies (typically in the MHz range) and power levels, the piezoelectric field generated by ultrasound in GaN adds an oscillating electric field component that can assist ionization of electrons from DX^- back to the conduction band. This can temporarily increase free-electron concentration and reduce compensation. Over prolonged exposure, strong ultrasonic fields can assist defect migration or annealing, promoting DX-to-shallow donor conversion or even structural healing of the local distortion.

Observable effects

Several measurable consequences have been reported or predicted:

- Changes in resistivity: Ultrasonic excitation can decrease resistivity in n -type GaN by releasing electrons trapped in DX centers.
- Altered luminescence intensity: PL or CL (cathodoluminescence) can show reversible intensity changes as the occupation of deep centers fluctuates.
- Acoustic attenuation and velocity changes: The interaction between DX centers and strain fields leads to characteristic temperature- and frequency-dependent attenuation peaks (acoustic relaxation).

- Persistent photoconductivity modulation: Ultrasonic waves can accelerate recovery from persistent photoconductivity by providing an alternative relaxation channel for metastable DX defects.

In short, ultrasonic vibrations affect DX centers by modulating strain, electric fields, and defect potential landscapes, leading to reversible changes in charge state, conductivity, and optical activity. This coupling between acoustics and defect dynamics is exploited in acoustic annealing experiments and in studies of lattice-defect energetics in GaN and AlGaN materials.

Effect of high-frequency (including terahertz) irradiation on properties of GaN with DX centers

High-frequency electromagnetic irradiation – including microwave, sub-terahertz, and terahertz (THz) ranges – can have marked effects on GaN containing DX centers, because these metastable donor defects couple strongly to both electric fields and lattice vibrations. The response depends on the field amplitude, photon energy, and the defect's configuration barrier (typically tens to hundreds of meV). Let's look at possible mechanisms of interaction:

a. Electric-field coupling (microwave to THz):

- DX centers involve a polar lattice distortion – the donor atom (e.g., Si_{Ga} or O_N) shifts off-center in its lattice site.
- Alternating electric fields from high-frequency radiation periodically polarize the lattice, modulating this off-center displacement.
- Strong fields can induce charge-state transitions ($DX^- \leftrightarrow d^0$) by field-assisted tunneling or ionization of the trapped electron into the conduction band.
- The ionization threshold corresponds to photon energies of about tens of meV ($\approx$ THz range), so THz radiation can resonantly excite bound electrons in shallow or metastable states.

b. Electron-heating mechanism:

- Under sub-bandgap irradiation (e.g., intense THz pulses), conduction electrons gain kinetic energy ("hot electrons") without generating new carriers by absorption.
- Hot electrons can thermally detrap from DX centers, raising the free electron concentration and transient conductivity.
- Relaxation after the pulse can reveal recovery kinetics of the DX state.

c. Phonon resonance and lattice coupling:

- Terahertz frequencies overlap with optical phonon modes.
- Intense THz fields can drive nonlinear phonon oscillations, locally altering the lattice potential around DX centers and transiently flattening or reshaping the energy barrier between shallow and deep configurations.

What are observable effects and phenomena in this case:

- Photoionization of DX centers: THz photons with ≥ 30 –100 meV energy can ionize deep donor electrons, similar to mid-IR radiation but without creating band-to-band transitions.

- Conductivity changes: Measured as transient increases in carrier density or THz transmission (time-domain THz spectroscopy).
- Metastability control: Repetitive THz exposure can depopulate DX⁻ centers, shifting material toward its shallow-donor configuration – effectively "*photo-annealing*" the metastable state.
- Luminescence modulation: Band-edge or deep-level PL intensity can change due to altered defect charge states.
- THz absorption signatures: DX-related transitions produce characteristic sub-bandgap absorption or relaxation peaks, useful for defect spectroscopy.

In Table IV, we compare the manifestation of different effects across frequency regimes.

Several practical applications of the effects discussed above can be suggested:

- Reversible control: Non-destructive tuning of donor occupation and compensation level *via* THz pulses.
- Characterization tool: THz time-domain spectroscopy can probe DX-related trap energies and capture/emission times.
- Potential degradation or annealing: Continuous high-intensity THz or microwave exposure could either stabilize the shallow configuration (reducing compensation) or, at excessive power, damage the lattice through overheating.

Summarizing this paragraph, the following conclusion can be drawn:

Terahertz and other high-frequency fields can dynamically control the electronic and structural state of DX centers in GaN by driving charge emission, lattice relaxation, and local polarization switching. These processes alter conductivity, optical emission, and metastability, offering both diagnostic and defect-engineering routes for wide-bandgap semiconductors.

Effect of DX centers on properties of plasmonic structures based on AlGaN/GaN heterostructures

DX centers in AlGaN/GaN heterostructures strongly influence the optical and electronic behavior of plasmonic structures, especially those exploiting the 2DEG (two-dimensional electron gas) at the interface as the plasmonic medium. Because plasmonic resonances in these systems depend sensitively on carrier density, scattering rates, and local permittivity, DX centers – acting as metastable donors and traps – affect both the strength and dynamics of plasmonic response.

First, we should consider the effects of the DX centers on the plasmonic response. DX centers in AlGaN (mainly Si_{Ga} or O_N) control how many electrons are donated to the 2DEG. When donors convert into DX⁻ states, fewer electrons populate the 2DEG, and the plasmon frequency decreases, and the intensity weakens. Under optical or high-field excitation, ionization of DX⁻ $\rightarrow$ d⁰ releases electrons, and the plasmon frequency blue-shifts and amplitude increases. This is the basis for photo- or bias-tunable plasmonic effects in GaN-based heterostructures.

Table IV.

Frequency range	Dominant interaction	Typical outcome
MHz–GHz (microwave)	Field-assisted tunneling, local heating	Minor conductivity modulation
0.1–3 THz	Photon-assisted ionization, electron heating, phonon coupling	$DX^- \rightarrow d^0$ conversion, photoconductivity rise
>10 THz (far-IR)	Resonance with LO-phonons, strong lattice coupling	Structural relaxation, possible persistent state change

Table V.

Property	DX-related influence	Experimental manifestation
THz plasmon resonance frequency	Red-shift when DX^- dominant; blue-shift after photoionization	Reversible tuning under UV/THz illumination
Linewidth / Q-factor	Increased due to carrier scattering	Broadened spectral response
Intensity (plasmon coupling strength)	Reduced by carrier depletion	Lower transmission/reflectance modulation
Time response / hysteresis	Slow recovery ($\sim$ s–min) due to trapped carriers	Memory effect in THz or IR modulation
Temperature dependence	Recovery of n_{2DEG} with heating ($DX^- \rightarrow d^0$ re-ionization)	Thermally activated resonance shift

Nonlinear and time-dependent behavior must also be considered. DX centers are metastable; transitions between charge states are slow (μ s–s scale). This produces plasmonic hysteresis and memory effects – plasmon resonances depend on illumination history or bias cycling. Illumination can produce persistent photoplasmonic conductivity, analogous to persistent photoconductivity, where plasmon resonances persist long after light is turned off.

Finally, two more important factors should be considered when analyzing experimental results. First, **mobility degradation**. Charged DX centers act as strong Coulomb scattering centers near the interface. They increase the electron scattering rate (τ), broadening and damping plasmon peaks. As Al content rises ($x > 0.4$), DX centers become deeper and more abundant, reducing the plasmonic quality factor $Q = \omega_p/\tau$. Second, **local permittivity and field uniformity**. Spatially inhomogeneous charge trapping at DX sites causes fluctuations in the local dielectric environment. This leads to plasmon resonance broadening and mode localization, particularly in nanostructured metasurfaces or gratings fabricated on AlGaIn/GaN. Table V summarizes observable consequences in this case.

In summary, DX centers in the AlGaIn barrier of plasmonic AlGaIn/GaN heterostructures act as metastable charge traps that dynamically control the 2DEG density, scattering rate, and local dielectric environment. They cause frequency shifts, intensity modulation, and damping of plasmon resonances, while also enabling persistent and reversible control *via* optical or electrical stimuli. This dual role makes DX centers both a source of loss and a potential mechanism for active tuning or memory in GaN-based plasmonic and terahertz devices.

What actions should be proposed to avoid the effects of metastable defects in III-nitride-based devices

Suppressing or mitigating the effects of metastable defects (like DX centers, vacancy complexes, or impurity-related traps) in III-nitride devices (GaN, AlGaIn, InGaIn, AlN) requires a combination of material engineering, process optimization, and device design strategies. The goal is to minimize defect formation, prevent their activation, and reduce their impact on charge transport, optical recombination, and long-term stability. Five steps are proposed to implement this task:

Step 1. Materials growth strategies

a. Optimize growth conditions

- Maintain near-stoichiometric conditions and low background impurity levels during MOCVD or MBE growth to minimize formation of nitrogen vacancies and unwanted dopant complexes.
- Avoid excessively high Al content and high pressure, which favor lattice relaxation leading to DX states in *n*-type dopants (especially Si and O).

b. Use alternative doping strategies

- Ge instead of Si for *n*-type doping: Ge donors stay shallower and show less DX tendency in AlGaIn with moderate Al fractions ($x < 0.6$).
- Minimize O and H contamination, which form metastable or amphoteric centers contributing to compensation.
- For *p*-type doping, control Mg–H complex formation (a metastable pair) through proper activation annealing.

Table VI.

Approach	Purpose	Key benefit
Low Al barrier or graded AlGaIn	Prevent DX formation	Stable 2DEG density
Ge doping (instead of Si)	Avoid DX centers	Shallow donor behavior
Post-growth anneal	Relax metastable configurations	Improve carrier activation
Controlled hydrogen management	Prevent metastable hydrogenic defects	Long-term stability
Field-management design	Reduce charge trapping	Mitigate current collapse
Optical pre-stimulation	Reset defective charge states	Stable initial operation

c. Heterostructure design adjustments

- Use lower Al composition (or graded Al profiles) in the barrier layers of AlGaIn/GaN heterostructures to stay below the DX transition threshold (typically 40–50% Al).
- Introduce spacer layers or undoped buffer regions to spatially separate dopant atoms from active regions (reduces trap scattering and charge transfer variability).

Step 2. Post-growth treatments

a. Thermal annealing

- Proper post-growth annealing (700–900 °C) helps convert metastable defect configurations back into their shallow donor states and remove hydrogen passivation.
- Multi-step anneals under nitrogen or ammonia can reduce vacancy complex density and stabilize dopant charge states.

b. UV or optical activation

- Controlled UV illumination can empty deep traps, restore free-carrier concentration, and “reset” devices before operation.
- Used cautiously, this can pre-stabilize the lattice and minimize drift during device use.

Step 3. Defect passivation and compensation control

- Deposit dielectric caps (SiN_x , Al_2O_3 , HfO_2) to suppress surface states that interact with internal metastable centers.
- Apply hydrogen control: while H can passivate defects, excess hydrogen introduces metastable Mg–H and donor–H complexes; carefully balance through annealing or plasma treatments.
- Introduce compensating dopants or co-doping schemes to reduce Fermi-level pinning that promotes DX conversion.

Step 4. Device and operational strategies

a. Limit high electric fields and bias stress

- Avoid prolonged high-field operation or bias stress that drives charge transfer into deep DX states.
- Design with field plates or graded barriers to lower peak fields around gate edges in HEMTs.

b. Stabilize thermal environment

- Thermal cycling enhances reconfiguration of metastable centers. Maintain steady operating temperatures or provide self-heating management via efficient thermal paths.

c. Preconditioning before use

- Controlled electrical or optical conditioning helps “fill” or “empty” traps in a predictable way, improving reproducibility.

Step 5. Characterization and feedback control

- Employ deep-level transient spectroscopy (DLTS), cathodoluminescence, and time-resolved photoconductivity to identify metastable traps and monitor their evolution during processing.
- Use this feedback to fine-tune growth and annealing parameters for each specific device structure.

Table VI summarizes the results of performing the steps listed above.

General conclusion:

The paper is a concise, structured review-style summary covering the main concepts, mechanisms, experimental signatures, theoretical approaches, and device implications. Actions that should be proposed to avoid the effects of metastable defects in III-nitride-based devices are discussed. Avoiding metastable defect effects in III-nitride devices requires preventing their formation (through growth and doping control), stabilizing their electronic configuration (by annealing or optical activation), and designing device architectures that minimize field- or temperature-induced transitions. These combined actions ensure consistent carrier density, higher mobility, and superior optical and electrical reliability in GaN-, AlGaIn-, and InGaIn-based devices. It is shown that suppressing or mitigating the effects of metastable defects (like DX centers, vacancy complexes, or impurity-related traps) in III-nitride devices (GaN, AlGaIn, InGaIn, AlN) requires a combination of material engineering, process optimization, and device design strategies. The goal is to minimize defect formation, prevent their activation, and reduce their impact on charge transport, optical recombination, and long-term stability.

Acknowledgments

This study was supported by the National Academy of Sciences of Ukraine (Project No. 5.2/26-II). A.E.B. gratefully acknowledges the long-term program supporting the Ukrainian research teams at the Polish Academy of Sciences, which was carried out in collaboration with the U.S. National Academy of Sciences with the financial support of external partners

(Project: LTP NAS KOCHELAP A7.11.0008; contract # PAN.BFB.S.BWZ.367.022.2023). The authors would also like to thank V.A. Kochelap and V.V. Koroteyev for the valuable collaborative work.

References

1. *GaN-Based Materials and Devices: Growth, Fabrication, Characterization and Performance*. Eds. M.S. Shur and R.F. Davis. World Scientific Publishing Co. Pte. Ltd., 2011. <https://doi.org/10.1142/5539>.
2. Morkoç H. *Nitride Semiconductors and Devices*. Springer Berlin, Heidelberg, 1999. <https://doi.org/10.1007/978-3-642-58562-3>.
3. Cai L., Feng C. Effect of vacancy defects on the electronic structure and optical properties of GaN. *J. Nanotechnol.* 2017. Art. ID 6987430. <https://doi.org/10.1155/2017/6987430>.
4. Uedono A., Iguchi H., Horita M. *et al.* Vacancy-type defects in *n*-type GaN fabricated by low-dose ion implantation studied by a monoenergetic positron beam. *phys. status solidi (b)*. 2025. **263**. P. e202500409. <https://doi.org/10.1002/pssb.202500409>.
5. Diallo I.C., Demchenko D.O. Native point defects in GaN: A hybrid-functional study. *Phys. Rev. Appl.* 2016. **6**. P. 064002. <https://doi.org/10.1103/PhysRevApplied.6.064002>.
6. Murakami F., Takeo A., Mitchell B. *et al.* Enhanced luminescence efficiency in Eu-doped GaN superlattice structures revealed by terahertz emission spectroscopy. *Commun. Mater.* 2023. **4**. 100. <https://doi.org/10.1038/s43246-023-00428-6>.
7. Mitchell B., Hernandez N., Lee D. *et al.* Charge state of vacancy defects in Eu-doped GaN. *Phys. Rev. B*. 2017. **96**. P. 064308. <https://doi.org/10.1103/PhysRevB.96.064308>.
8. Wang J., Koizumi A., Fujiwara Y., Jadwisieniczak W.M. Study of defects in GaN *in situ* doped with Eu³⁺ ion grown by OMVPE. *J. Electron. Mater.* 2016. **45**. P. 2001–2007. <https://doi.org/10.1007/s11664-016-4337-4>.
9. Chaulker O.H., Turkulets Y., Shalish I. The Mg related GaN blue luminescence deep level and its connection to an MgO surface state. *Sci. Rep.* 2025. **15**. P. 18773. <https://doi.org/10.1038/s41598-025-97446-w>.
10. Kumar A., Berg M., Wang Q. *et al.* Acceptor activation of Mg-doped GaN – Effects of N₂/O₂ vs N₂ as ambient gas during annealing. *J. Appl. Phys.* 2023. **134**. P. 035701. <https://doi.org/10.1063/5.0139114>.
11. Duc T.T., Pozina G., Amano H. *et al.* Deep level study of Mg-doped GaN using deep level transient spectroscopy and minority carrier transient spectroscopy. *Phys. Rev. B*. 2016. **94**. P. 045206. <https://doi.org/10.1103/PhysRevB.94.045206>.
12. Lang D.V. DX centers in III-V alloys, Ch. 7, in: *Deep Centers in Semiconductors*. Ed. S.T. Pantelides. Gordon & Breach Science Publ., 1992. P. 489–539. <https://doi.org/10.1201/9781003580409>.
13. Wetzel C., Suski T., Ager III J.W. *et al.* Pressure induced deep gap state of oxygen in GaN. *Phys. Rev. Lett.* 1997. **78**. P. 3923. <https://doi.org/10.1103/PhysRevLett.78.3923>.
14. McCluskey M.D., Johnson N.M., Van de Walle C.G. *et al.* Metastability of oxygen donors in AlGaIn. *Phys. Rev. Lett.* 1998. **80**. P. 4008. <https://doi.org/10.1103/PhysRevLett.80.4008>.
15. Skierbiszewski C., Suski T., Leszczynski M. *et al.* Evidence for localized Si-donor state and its metastable properties in AlGaIn. *Appl. Phys. Lett.* 1999. **74**. P. 3833. <https://doi.org/10.1063/1.124195>.
16. Gorczyca I., Suski T., Perlin P. *et al.* Hydrostatic pressure as a tool for the study of semiconductor properties – An example of III–V nitrides. *Materials*. 2024. **17**. P. 4022. <https://doi.org/10.3390/ma17164022>.
17. Collazo R., Mita S., Xie J. *et al.* Progress on *n*-type doping of AlGaIn alloys on AlN single crystal substrates for UV optoelectronic applications. *phys. status solidi (c)*. 2011. **8**. P. 2031. <https://doi.org/10.1002/pssc.201000964>.
18. Bryan I., Bryan Z., Washiyama S. *et al.* Doping and compensation in Al-rich AlGaIn grown on single crystal AlN and sapphire by MOCVD. *Appl. Phys. Lett.* 2018. **112**. P. 062102. <https://doi.org/10.1063/1.5011984>.
19. Borisov B., Kuryatkov V., Kudryavtsev Y. *et al.* Si-doped layers grown by molecular beam epitaxy with ammonia. *Appl. Phys. Lett.* 2005. **87**. P. 132106. <https://doi.org/10.1063/1.2061856>.
20. Brandt M.S., Zeisel R., Gönnenwein S.T.B. *et al.* DX behaviour of Si donors in AlGaIn alloys. *phys. status solidi (b)*. 2003. **235**. P. 13–19. <https://doi.org/10.1002/pssb.200301521>.
21. Bagheri P., Kirste R., Reddy P. *et al.* The nature of the DX state in Ge-doped AlGaIn. *Appl. Phys. Lett.* 2020. **116**. P. 222102. <https://doi.org/10.1063/5.0008362>.
22. Yan Q., Lyons J.L., Gordon L. *et al.* Oxygen impurities in AlN and their impact on optical absorption. *Appl. Phys. Lett.* 2025. **126**. P. 062106. <https://doi.org/10.1063/5.0234655>.
23. Gordon L., Lyons J.L., Janotti A., Van de Walle C.G. Hybrid functional calculations of DX centers in AlN and GaN. *Phys. Rev. B* 2014. **89**. P. 085204. <https://doi.org/10.1103/PhysRevB.89.085204>.
24. Özkişi H., Özkapı B., Özkapı S.G., Dalgıç S. Electronic band structures of Te-doped GaN nanowires. *Mater. Today Proc.* 2017. **4**, No 11. P. 11640–11643. <https://doi.org/10.1016/j.matpr.2017.09.076>.
25. Ardakani Y.S., Moradi M. Electronic and optical properties of Te-doped GaN monolayer before and after adsorption of dimethylmercury – DFT+U/TDDFT & DFT-D2 methods. *J. Mol. Graph. Model.* 2021. **104**. P. 107837. <https://doi.org/10.1016/j.jmgm.2021.107837>.
26. Park C.H., Chadi D.J. Stability of deep donor and acceptor centers in GaN, AlN, and BN. *Phys. Rev. B*. 1997. **55**, No 19. P. 12995. <https://doi.org/10.1103/PhysRevB.55.12995>.

27. Tien N.S., Bickermann M., Janzén E. Shallow donor and DX states of Si in AlN. *Appl. Phys. Lett.* 2011. **98**. P. 092104. <http://doi.org/10.1063/1.3559914>.
28. Szafranski B., Peters L., Wolter S. *et al.* Ionization energy of the oxygen donor in AlN. *Appl. Phys. Lett.* 2026. **128**. P. 042101. <http://doi.org/10.1063/5.0308036>.
29. Yan Q., Lyons J.L., Gordon L. *et al.* Oxygen impurities in AlN and their impact on optical absorption. *Appl. Phys. Lett.* 2025. **126**. P. 062106. <http://doi.org/10.1063/5.0234655>.
30. Forbus J., Wickramaratne D., Lyons J.L., Zvanut M.E. Nonradiative quenching of EPR signals in germanium-doped AlGaIn: Evidence for DX-center formation. *Appl. Phys. Lett.* 2025. **126**. P. 042101. <http://doi.org/10.1063/5.0249701>.

Author and CV



Alexander Belyaev, Doctor of Sciences in Physics and Mathematics, Professor, Academician of the NAS of Ukraine. He is the author of more than 240 publications. The area of his scientific activity is transport in quantum multilayer heterostructures and low-dimensional systems and their optical properties, as well as the application of such structures in UHF devices. <https://orcid.org/0000-0001-9639-6625>

Метастабільні дефекти в III-нітридах

О.Є. Беляєв

Анотація. Метастабільні стани в III-нітридах (AlN, GaN, InN та їхні сплави) є важливою темою в матеріалознавстві, фізиці приладів та епітаксимальному вирощуванні, оскільки ці сполуки демонструють численні конкуруючі кристалічні структури, конфігурації дефектів та фазову поведінку, які сильно впливають на оптичні, електричні та механічні властивості. Стаття являє собою стислий, структурований оглядовий виклад, що охоплює основні концепції, механізми, експериментальні прояви, теоретичні підходи та значення для приладів. Обговорюються дії, які слід запропонувати, щоб уникнути впливу метастабільних дефектів у пристроях на основі III-нітридів. Уникнення ефектів метастабільних дефектів у пристроях на основі III-нітридів вимагає запобігання їх утворенню (шляхом контролю росту та легування), стабілізації їхньої електронної конфігурації (шляхом відпалу або оптичної активації) та проєктування архітектур приладів, які мінімізують переходи, індуковані полем або температурою. Ці комбіновані дії забезпечують необхідну густину носіїв заряду, вищу рухливість та чудову оптичну і електричну надійність у пристроях на основі GaN, AlGaIn та InGaIn.

Ключові слова: метастабільні дефекти, III-нітриди, електронна конфігурація, переходи, викликані полем або температурою.