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Probing quantum defect states in Zr-doped homoepitaxial AlN

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ABSTRACT

The neutral defect complex comprising zirconium substituting onto the Al sublattice (Zr_{Al}) and an adjacent nitrogen vacancy (V_{N}), $(\text{Zr}_{\text{Al}}-\text{V}_{\text{N}})^0$, in aluminum nitride (AlN) crystals is theoretically predicted to host unique spin states suitable for quantum manipulation. Here, we report experimental observations of both intradefect and band-to-impurity optical transitions involving $(\text{Zr}_{\text{Al}}-\text{V}_{\text{N}})^0$ in AlN. This defect was realized via *in situ* doping of Zr into AlN homoepitaxial layers grown by metalorganic chemical vapor deposition. Below-bandgap excitation at $\lambda_{\text{exc}} = 260$ nm resolved emission peaks at 1.89, 2.11, and 3.52 eV, in excellent agreement with those predicted by first-principles calculations for the intradefect and band-to-impurity type of transitions involving $(\text{Zr}_{\text{Al}}-\text{V}_{\text{N}})^0$, providing experimental validation of the defect's electronic structure. Temperature-dependent PL further demonstrates that the $(\text{Zr}_{\text{Al}}-\text{V}_{\text{N}})^0$ state maintains a stable optical emission up to room temperature, with a high thermal activation energy of 48 meV, indicative of thermal robustness against nonradiative quenching. While further spin-based measurements are needed to assess coherence and manipulation limits, experimental and theoretical findings validate Zr-doped AlN as a promising platform for the realization of room-temperature quantum defect devices, including solid-state qubits and integrated quantum photonic technologies.

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AlN has emerged as a highly promising crystalline host for solid-state quantum defects¹ due to its exceptional combination of electrical, optical, and material properties, including an ultra-wide bandgap (UWBG) of about 6.1 eV,² relatively weak spin-orbit coupling,³ availability of high crystalline quality bulk crystals for homoepitaxial growth,^{4–7} excellent thermal conductivity,^{8,9} strong piezoelectric response,¹⁰ and compatibility with established III-nitride optoelectronic device technologies.^{11–15} Collectively, these characteristics make AlN an attractive platform for hosting optically addressable quantum defects capable of operating under ambient conditions while remaining compatible with scalable semiconductor device fabrication.

Several defects in AlN have been investigated as potential solid-state qubits^{1,16–18} and transition metal impurities have been found to offer considerable potential, since they can introduce highly localized electronic defect states within the wide bandgap that are sufficiently stable and have modest formation energies.¹ Theoretical¹ and experimental studies^{16–20} have identified zirconium (Zr) as a favorable transition metal dopant that preferentially substitutes on the Al lattice site (Zr_{Al}) and acts as a deep donor impurity that may be of a simple defect state or form complex defects within AlN. Of particular interest is the neutral Zr–N vacancy complex, $(\text{Zr}_{\text{Al}}-\text{V}_{\text{N}})^0$, which is predicted to support localized quantum states that are energetically

decoupled from delocalized conduction band states.¹ Such electronic isolation is expected to minimize interactions with the host lattice, thereby suppressing decoherence pathways and enabling long-lived quantum states, making the $(\text{Zr}_{\text{Al}}-\text{V}_{\text{N}})^0$ defect particularly attractive.

However, experimental validation of calculated optical transition energies and definitive identification of the associated defect states remains challenging. Previous studies relied on ion implantation for Zr incorporation,^{18,19} or *in situ* doping during heteroepitaxial growth on sapphire substrate for obtaining Zr-doped AlN (AlN:Zr) thin films.^{19,20} Although these approaches successfully introduce Zr into the AlN lattice, they can also generate significant concentrations of structural defects, impurities, and strain-induced disorders arising from implantation damage or lattice mismatch. This extrinsic defect population produces competing optical emissions and broadened spectroscopic features, which obscures the comparative signatures associated with Zr-related quantum defect states. As a result, direct experimental observation and unambiguous assignment of the theoretically predicted optical transitions associated with the $(\text{Zr}_{\text{Al}}-\text{V}_{\text{N}})^0$ defect center remained elusive.

In this work, we present an experimental investigation on Zr-doped homoepitaxial AlN films grown via metalorganic chemical

vapor deposition (MOCVD), with the aim to identify the optical transitions associated with Zr-related defects. The enhanced crystalline quality of AlN:Zr films afforded by homoepitaxial growth provides an ideal platform for probing the intrinsic Zr-related optical transitions while minimizing interference from extrinsic defects and strain-induced disorders. Photoluminescence (PL) spectroscopy was employed to probe defect-mediated optical processes under both above- and below-bandgap excitation conditions. The measured emission features are directly compared to a reference undoped sample and interpreted in conjunction with first-principles calculations for Zr-related defect optical transitions. Temperature dependent PL spectroscopy was also performed to evaluate the thermal stability and activation behavior of the Zr-related emissions.

Undoped and Zr-doped AlN epilayers were grown by MOCVD on 2-in. diameter AlN bulk substrates grown by physical vapor transport (PVT) (by Crystal IS). Trimethylaluminum (TMA) and ammonia (NH_3) were utilized as the Al and N precursors, respectively. *In situ* Zr doping was achieved using tetrakis (dimethylamino) zirconium $\{\text{TDMAZr}, \text{Zr}[\text{N}(\text{CH}_3)_2]_4\}$ as a Zr precursor using hydrogen as the carrier gas. The undoped and Zr-doped epilayers used in this study had thicknesses of approximately $10\ \mu\text{m}$ as determined by profilometry. Secondary ion mass spectrometry (SIMS) depth profiling was utilized to quantify dopant concentration and compositional uniformity. Structural quality was evaluated using high-resolution x-ray diffraction (HR-XRD) through rocking curve (ω -scan) measurements of the AlN (002) diffraction peak. For PL characterization, a femtosecond (fs) Ti:Sapphire laser operating at 76 MHz was utilized as a laser excitation source. The 780 nm (1.59 eV) laser output was frequency-

quadrupled to achieve a laser output at $\lambda_{\text{exc}} = 195\ \text{nm}$ (6.35 eV) with an average optical power of 1 mW to provide an above-bandgap excitation, whereas the frequency-tripled laser output ($\lambda_{\text{exc}} = 260\ \text{nm}$, 4.77 eV) with an average power output of 5 mW was utilized for a below-bandgap excitation. The PL detection system consisted of a 1.3 m monochromator coupled to a micro-channel plate photomultiplier tube (MCP-PMT), covering a spectral range of 200–800 nm. Temperature-dependent measurements were conducted between 10 and 300 K in a closed-cycle helium cryostat.

Figure 1(a) shows the SIMS depth profile analysis of the Zr-doped AlN (AlN:Zr) homoepitaxial sample, revealing a homogeneous Zr concentration of $3.3 \times 10^{19}\ \text{cm}^{-3}$ within the AlN matrix. The crystalline quality of AlN undoped and Zr-doped AlN epilayers was evaluated using HR-XRD ω -rocking scans of the AlN (002) diffraction peak. As shown in Fig. 1(b), both samples exhibit sharp and symmetric diffraction peaks. The undoped reference sample exhibits a full width at half maximum (FWHM) of 22 arc sec, representative of the exceptional crystalline quality attainable in homoepitaxial AlN. A significant challenge for obtaining high-quality AlN:Zr epilayers is to manage the atomic size difference between Zr and Al, which introduces a substantial lattice mismatch between the AlN:Zr epilayer and the AlN bulk substrate. Our recent work has shown that by inserting a graded doping transition layer between the top AlN:Zr active layer and the AlN bulk substrate, strain accumulation at the AlN:Zr/AlN interface and within the AlN:Zr epilayer can be effectively suppressed.²¹ By adopting this graded doping transition layer strategy, the rocking curve of the resultant AlN:Zr epilayer broadens only modestly to 74 arc sec. Although this increase indicates the

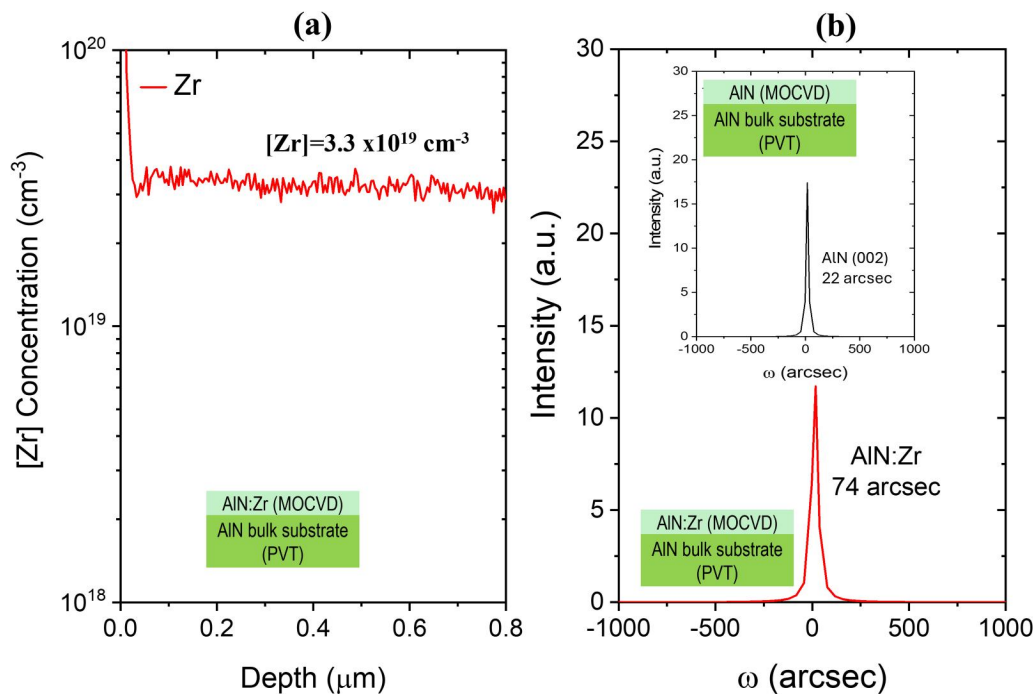


FIG. 1. (a) Zr concentration in a Zr-doped AlN (AlN:Zr) homo-epilayer grown by MOCVD measured using SIMS. The schematic layer structure is shown in the inset. (b) XRD (002) rocking curve (ω -scan) of a Zr-doped AlN (AlN:Zr) homo-epilayer. The comparison XRD (002) rocking curve of a reference undoped AlN homo-epilayer sample is shown in the inset.

introduction of additional crystalline disorder upon Zr incorporation, the narrow linewidth confirms that the overall structural quality of AlN:Zr epilayer remains excellent.

It is worth noting that the structural quality achieved in the present work represents a substantial improvement over previously reported Zr-doped AlN films that have grown under less favorable conditions. In an earlier study of heteroepitaxial AlN:Zr grown on sapphire substrates, the AlN (002) rocking curve exhibited a FWHM of 216 arc sec¹⁹ at a comparable Zr concentration, reflecting the additional crystalline imperfections associated with lattice mismatch and heteroepitaxial strain. Even larger degradation has been reported for Zr incorporation by ion implantation, where rocking curve widths of approximately 1.4° have been observed,¹⁷ indicative of extensive implantation-induced lattice damage. The significantly narrower XRD rocking curve obtained for the homoepitaxial MOCVD grown AlN:Zr films demonstrates that *in situ* doping during homoepitaxial growth in conjunction with the graded doping transition layer approach provides an effective route for incorporating Zr while preserving crystalline quality. The combination of a homogeneous Zr distribution and excellent crystalline quality makes detailed optical investigations possible. Reduced structural disorder minimizes competing defect-related luminescence and inhomogeneous broadening, thereby enabling more reliable identification of optical transitions originating from the predicted $(\text{Zr}_{\text{Al}} - \text{V}_{\text{N}})^0$ quantum defect complex.

Figure 2 presents the low-temperature (10 K) photoluminescence (PL) spectra of the undoped AlN and AlN:Zr homoepitaxial samples under above-bandgap excitation ($\lambda_{\text{exc}} = 195 \text{ nm}$). A schematic illustration of the PL measurement configuration is shown in Fig. 2(a). The PL spectrum of the undoped AlN reference sample, shown in the bottom panel of Fig. 2(b), is dominated by a sharp band

edge emission centered at 5.96 eV. The narrow linewidth and strong intensity of this feature indicate efficient excitonic recombination and confirm the excellent optical quality of the undoped AlN reference homoepitaxial film. Emissions from deep-level defects are observable but very weak, suggesting a relatively low concentration of optically active native defects within the undoped material. In contrast, as shown in the top panel of Fig. 2, the band edge emission is strongly quenched following Zr incorporation, while a broad deep-level emission band centered near 3.9 eV becomes the dominant spectral feature in the AlN:Zr sample. The introduction of Zr evidently modifies the recombination dynamics within the AlN host since photo-generated carriers are efficiently captured by defect-related states before radiative band edge recombination occurs. The broad band has been previously attributed to the recombination of electrons from the conduction band (or a shallow donor level) with holes trapped at deep-level acceptor states composed of aluminum vacancy (V_{Al})-oxygen (O_{N}) complexes.^{22–25} This band routinely shifts from 3.4 to 4 eV due to the coexistence of varying oxygen complex configurations with varying charge states, such as $(\text{V}_{\text{Al}} - 2\text{O}_{\text{N}})^{0/1-2-}$ and $(\text{V}_{\text{Al}} - \text{O}_{\text{N}})^{0/1-2-}$.^{22–24} Furthermore, these defect complexes are known to stabilize in two structural configurations, namely a π -bond configuration parallel to the *c* axis and a σ -bond configuration along the three equivalent basal plane bonds.^{25–28} Because this native defect recombination dominates the spectrum under above-bandgap excitation, the localized intradefect transitions of the dopant cannot be resolved under above-bandgap excitation.

PL studies were carried out under below-bandgap excitation ($\lambda_{\text{exc}} = 260 \text{ nm}$) to suppress dominant native defect transitions observed in the above-bandgap excitation scheme. The resulting PL spectra measured at 10 K are presented in Fig. 3 for both the Zr-doped and undoped AlN homoepitaxial samples. Both samples display a distinct emission peak at 2.64 eV, allowing us to definitively exclude its origin as being Zr related. In fact, this emission line has been frequently observed in AlN and has been typically associated with isolated $\text{V}_{\text{Al}}^{2-/3-}$ defect.²⁴ Similarly, a peak at 3.64 eV is observed in the undoped AlN sample, which can be attributed to sharing a common origin with the $(\text{V}_{\text{Al}} - \text{O}_{\text{N}})$ defect complexes responsible for the broad deep-level luminescence observed under above-bandgap excitation in the doped sample. Under below-bandgap excitation, only a subset of these defect states is efficiently excited, resulting in a considerably narrower emission feature compared with the broad 3.9 eV band shown in Fig. 2.

In contrast, the AlN:Zr sample displays three distinct optical signatures at 1.89, 2.11, and 3.52 eV that are absent in the undoped reference AlN sample. The exclusive appearance of these transitions following Zr incorporation provides compelling experimental evidence that their origins are due to Zr-induced defect states rather than native point defects in the AlN host. Furthermore, the relatively narrow linewidths of the 1.89 and 2.11 eV peaks indicate that they arise from discrete, localized electronic states rather than broad defect bands. As summarized in Table I, these measured transition energy lines exhibit remarkable alignment with first-principles calculations for the Zr-related quantum defects in AlN. The emission observed at 1.89 eV agrees well with the predicted 1.91 eV optical transition associated with $(\text{Zr}_{\text{Al}} - \text{V}_{\text{N}})^0$. The theoretical model suggests that this transition represents an intradefect spin-conserving excitation ($\text{S} \rightarrow \text{S}$) where both the initial and final electronic states remain localized

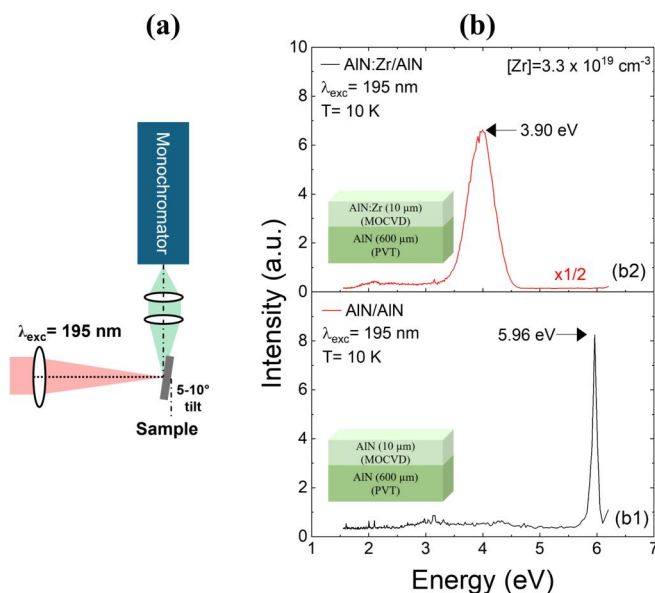


FIG. 2. (a) Schematic experimental setup for PL spectroscopy measurements. (b) Low temperature ($T = 10 \text{ K}$) PL emission spectra of undoped AlN (bottom panel) and AlN:Zr (top panel) homo-epilayers obtained under above-bandgap excitation ($\lambda_{\text{exc}} = 195 \text{ nm}$).

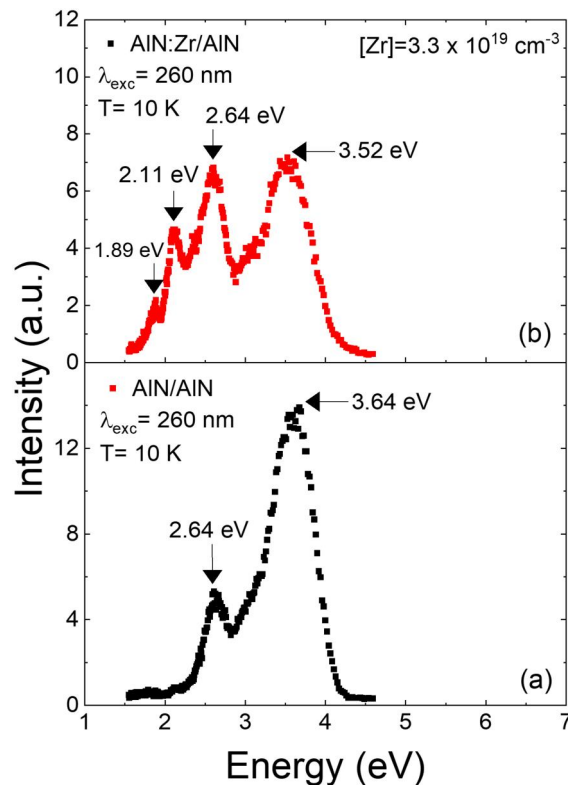


FIG. 3. Low-temperature (10 K) PL spectra of undoped AlN and AlN:Zr homoeplayers obtained under below-bandgap excitation ($\lambda_{\text{exc}} = 260$ nm), highlighting the distinct Zr-induced states.

within the defect while preserving the total spin multiplicity.¹ Such spin-conserving optical transitions are particularly interesting because they form the basis for spin-selective optical initialization and readout schemes employed in many solid-state quantum defect platforms.

The experimentally observed 3.52 eV emission coincides with the calculated intradefect transition energy associated with V_N^{-1}/V_N^{-2} defect. Despite sharing spin-conserving dynamics with the 1.89 eV peak, the V_N^{-1}/V_N^{-2} defect was identified to have a low energy potential difference between its high and low spin states and very close proximity to the CBM.¹ This limits its utility in quantum applications due to possible sensitivity to spin flips during potential quantum applications or decoherence due to coupling with bulk conduction

band states.¹ The peak at 3.52 eV appears broader than other peaks observed in the spectrum, which suggests that it may consist of multiple transitions, one of which may be the 3.64 eV peak observed in the undoped sample. Despite its broad nature, the 3.52 eV peak can be confidently assigned to $V_N^{-1/-2}$ defect transition, supported by its clear redshift relative to the 3.64 eV peak and excellent agreement with the predicted value, providing further support for the theoretical description of the defect-related electronic structure.¹ The remaining emission line observed at 2.11 eV in Fig. 3 corresponds to a band-to-impurity transition, where a conduction electron recombines with $(\text{Zr}_{\text{Al}} - \text{V}_\text{N})^+$ after an electron bound to the $(\text{Zr}_{\text{Al}} - \text{V}_\text{N})^0$ complex being promoted directly to the conduction band minimum (CBM) with a required optical ionization threshold of 3.07 eV.¹ The first-principles calculations further identify this process as a spin-majority transition ($S \rightarrow S - 1/2$), where electron emission into the conduction band changes the total spin of the defect by one-half. Consequently, the observation of this transition directly confirms the energetic position of the defect level relative to the host conduction band and indirectly provides valuable experimental support regarding the predicted spin-resolved electronic structure of the Zr-related quantum defect.

It is worth noting that the predicted spin-minority excitation of the $(\text{Zr}_{\text{Al}} - \text{V}_\text{N})^0$ complex with an optical emission at 3.78 eV was not observed in the spectrum shown in Fig. 3(b). This is because this transition has an optical ionization threshold of 4.97 eV,¹ which exceeds the 4.77 eV photon energy provided by the 260 nm excitation source. Although not all theoretically predicted transitions are experimentally resolved, the quantitative agreement between the measured and calculated transition energies, together with the absence of these emissions in the undoped reference sample, provides compelling experimental validation of the predicted Zr-related defect states.

The temperature evolution of the PL emission spectra under 260 nm excitation is presented in Fig. 4. The spectra were acquired over the temperature range of 10–300 K to investigate the thermal stability of the optical transitions associated with the Zr-related defect complexes. No significant shift in the emission energies is observed as the temperature increases, indicating that the optical transitions originate from stable defect configurations rather than thermally activated structural transformations or charge-state conversions. The emission centered at 3.52 eV attributed to the spin-conserving intradefect transition, $V_N^{-1/-2}$, decreases rapidly and becomes difficult to resolve above approximately 150 K. This rapid thermal quenching indicates that the excited state associated with the isolated $V_N^{-1/-2}$ readily couples to thermally activated nonradiative recombination pathways, limiting its optical stability at elevated temperatures. Meanwhile, the signatures at 1.89 and 2.11 eV associated with the $(\text{Zr}_{\text{Al}} - \text{V}_\text{N})^0$ complex remain

TABLE I. Comparison between calculated and experimentally measured optical emission energies associated with the spin-conserving excitations involving $(\text{Zr}_{\text{Al}} - \text{V}_\text{N})$ defect complex and V_N^{-1} defect in Zr-doped AlN. The competing channel that ionizes the $(\text{Zr}_{\text{Al}} - \text{V}_\text{N})^0$ defect center to the conduction band is also included. D^q represents the defect center D at a charge state q . All values are in eV.

	$D^q + \hbar\omega \rightarrow D^q$ Spin-conserving excitation: $S \rightarrow S$ (Emission)		$D^q + \hbar\omega \rightarrow D^{q+1} + e^- _{\text{CBM}}$ Spin-majority excitation: $S \rightarrow S - 1/2$ (Emission)	
	Calculated (Ref. 1)	Observed (This work)	Calculated (Ref. 1)	Observed (This work)
$(\text{Zr}_{\text{Al}} - \text{V}_\text{N})^0$ (eV)	1.91	1.89	2.11	2.11
V_N^{-1} and V_N^{-2} (eV)	3.52	3.52		

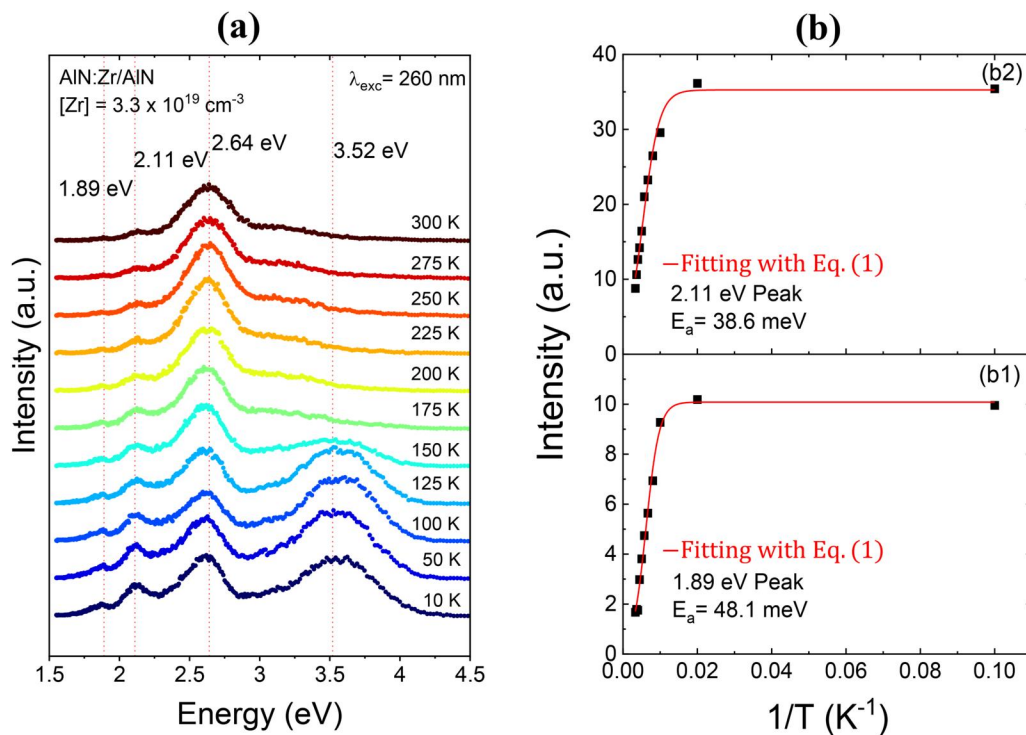


FIG. 4. (a) Temperature-dependent PL spectra (10–300 K) of AlN:Zr homo-epilayer under 260 nm excitation. (b) The corresponding Arrhenius plots of Eq. (1) for the emission intensities of (b1) the 1.89 eV emission and (b2) the 2.11 eV emission.

observable throughout the investigated temperature range. Although gradual thermal quenching is evident, both the 1.89 and 2.11 eV transitions retain substantial emission intensity, demonstrating greater thermal robustness than the isolated $V_N^{-1/-2}$. The persistence of these optical signatures suggests that the electronic states associated with the Zr-related defect complex are comparatively well isolated from thermally activated nonradiative recombination channels.

To quantitatively evaluate the thermal stability of the observed transitions, the integrated PL intensities of the 1.89 and 2.11 eV emission peaks were extracted as functions of temperature and analyzed using a single-activation-energy Arrhenius model,

$$I(T) = \frac{I_0}{1 + A \exp(-E_a/k_B T)}, \quad (1)$$

where I_0 is the low-temperature emission intensity, A is a fitting constant, k_B is Boltzmann's constant, and E_a represents the thermal activation energy associated with the dominant nonradiative quenching mechanism. The corresponding Arrhenius fits are presented in Figs. 4(b1) and 4(b2). Excellent agreement between the experimental data and the fitted curves is obtained over the full temperature range, indicating that the thermal quenching behavior of both transitions is well described by a single dominant activation process. The extracted activation energies for the 1.89 eV intradefect transition and the 2.11 eV band-to-impurity transition were determined to be 48 and 39 meV, respectively. The slightly lower activation energy for the band-to-impurity transition is consistent with its stronger interaction with extended conduction band states, making it somewhat susceptible to

thermally activated carrier escape and nonradiative relaxation. In comparison, the larger activation energy associated with the intradefect transition indicates that greater thermal energy is required to activate competing nonradiative recombination pathways. The persistence of the intradefect optical transitions up to room temperature, together with its relatively large activation energy, provides strong evidence that the defect retains stable radiative recombination under ambient conditions. This behavior is consistent with the theoretically predicted localization of the defect electronic states within the AlN bandgap and suggests that the defect remains largely decoupled from dominant nonradiative recombination channels. Although additional spin-based measurements will ultimately be required to evaluate quantum coherence and spin-manipulation capabilities, the demonstrated room-temperature optical emission stability satisfies a foundational benchmark for the development of Zr-related quantum defects in AlN for solid-state qubits and integrated quantum photonic applications. Additionally, Zr doping in AlN inherently drives the formation of nitrogen vacancies for charge compensation. Because the formation of $(Zr_{Al} - V_N)^0$ defects requires nitrogen vacancies adjacent to Zr donors, thermal annealing could boost their formation and associated optical signatures, a possibility that warrants further investigation.

In summary, we have synthesized high-quality undoped and Zr-doped AlN epilayers via homoepitaxial growth by MOCVD. Chemical composition and crystalline quality measurements confirmed incorporation of Zr into the intentionally doped AlN sample with minimum degradations in crystalline and optical qualities. PL

emission spectra under below-bandgap excitation resolved distinct emissions that were not present in the undoped AlN reference sample and which closely match the predicted electronic signature of the neutral $(\text{Zr}_{\text{Al}} - \text{V}_{\text{N}})^0$ defects. The thermal stability of the $(\text{Zr}_{\text{Al}} - \text{V}_{\text{N}})^0$ emission lines up to room temperature indicates that the defect states are well isolated and exhibit reduced susceptibility to thermally activated nonradiative recombination. These results provide important experimental validation of the predicted properties of Zr-related defects in AlN and establish homoepitaxial AlN as an ideal crystalline host capable of accommodating deep, decoupled quantum defect states.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

T. Njuguna: Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Software (equal); Validation (equal); Visualization (equal); Writing – original draft (equal). **H. Alwan:** Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Software (equal); Validation (equal); Visualization (equal); Writing – original draft (equal). **J. Li:** Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Software (equal); Supervision (equal); Validation (equal); Visualization (equal). **J. Y. Lin:** Conceptualization (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **H. X. Jiang:** Conceptualization (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available within the article.

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