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Electronic Supplementary Information

AlN interlayer-induced reduction of dislocation density in the AlGaN epilayer

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S1. HR-TEM characterisation

The GaN layer, in the heterostructure **A**, exhibits a thickness of approximately 2.2 µm, with dislocations evident in the corresponding dark-field image (Figure S2a), consistent with HR-XRD and CL findings (these latter are described below). Adjacent to the surface, the STEM-HAADF image distinctly reveals the AlGaN layer, characterised by a uniform thickness of 28.6 nm (Figure S2b), consistent with HR-XRD and XRR analyses. Figure S3 shows the STEM analyses assessed on heterostructure **C** at low magnification. The GaN layer is approximately 2 µm thick. Near the surface, the STEM-HAADF image highlights the presence of the AlGaN layer measuring approximately 18 nm in thickness, in good accordance with measurements obtained through HR-XRD and XRR techniques.

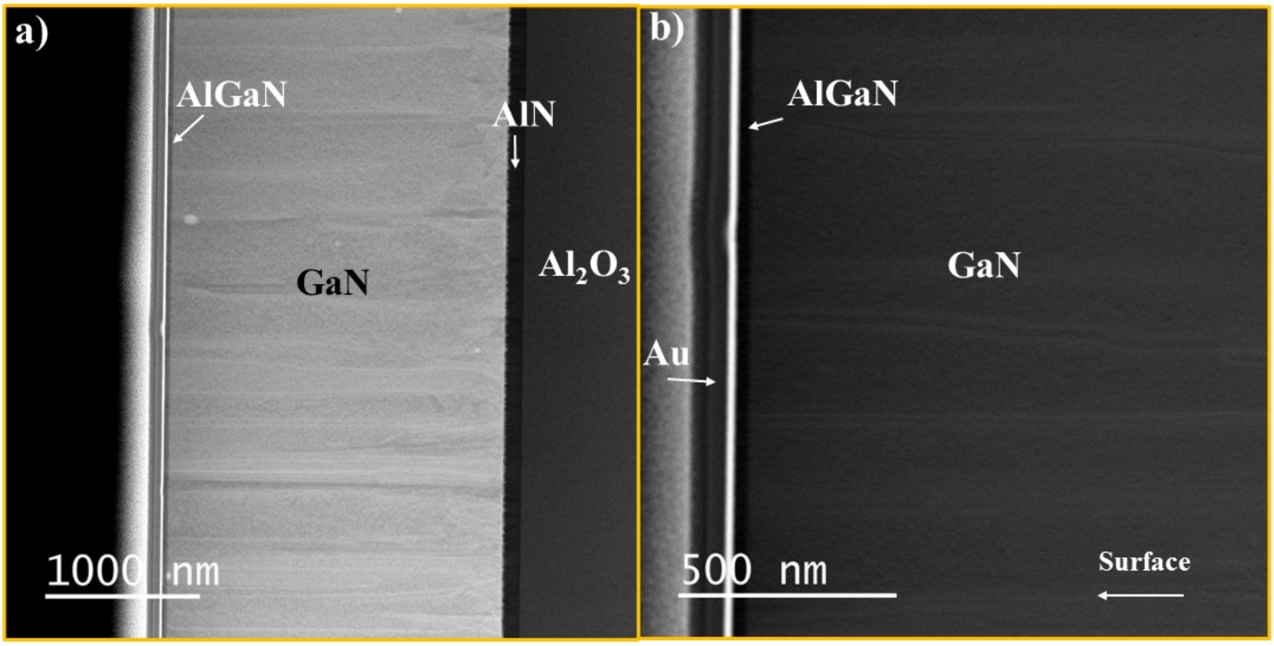

Figure S1 − (S)TEM analyses of the sample **A**: a) low-magnification STEM-HAADF image, b) low-magnification STEM-HAADF image showing the surface of the sample.

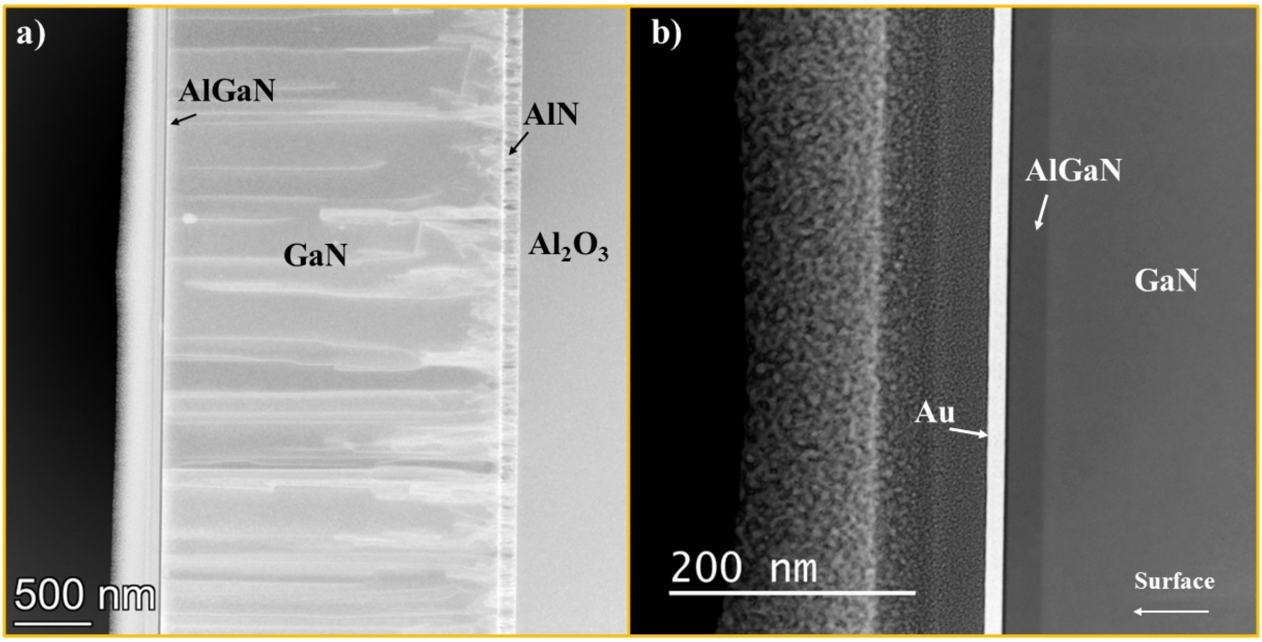

Figure S2 – (S)TEM analyses of the sample **A**: a) low-magnification STEM-DF image, b) medium-magnification STEM-HAADF image showing the surface of the sample.

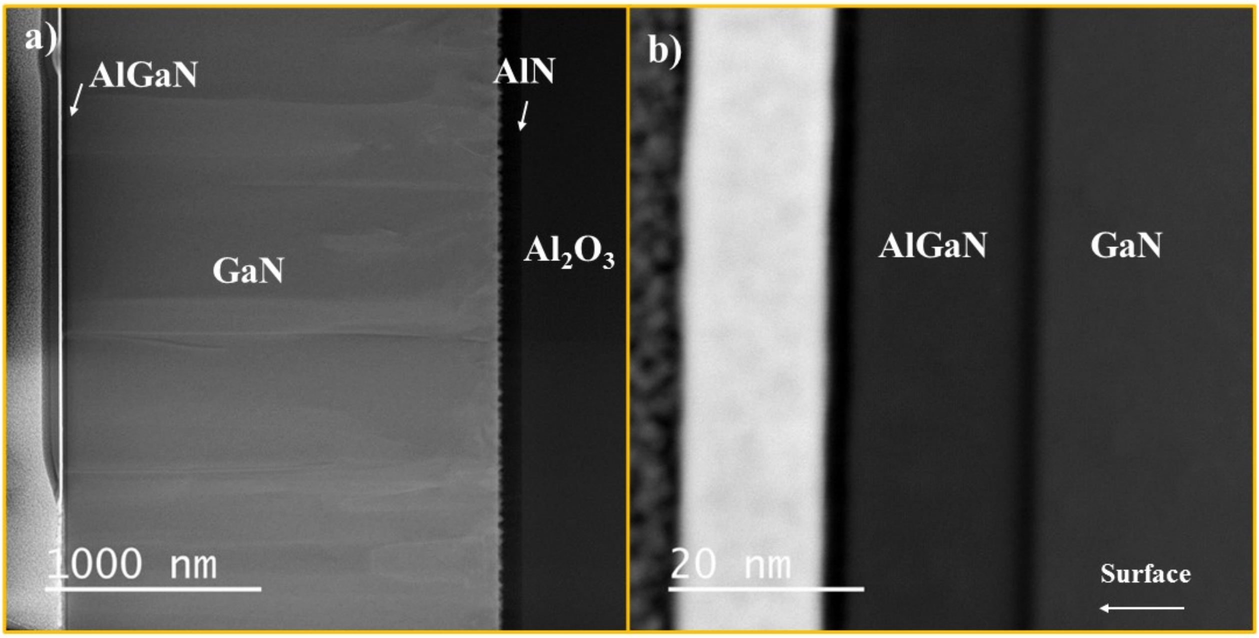

Figure S3 – (S)TEM analyses of the sample **C**: a) low magnification STEM-HAADF image, b) medium magnification STEM-HAADF image showing the surface of the sample.

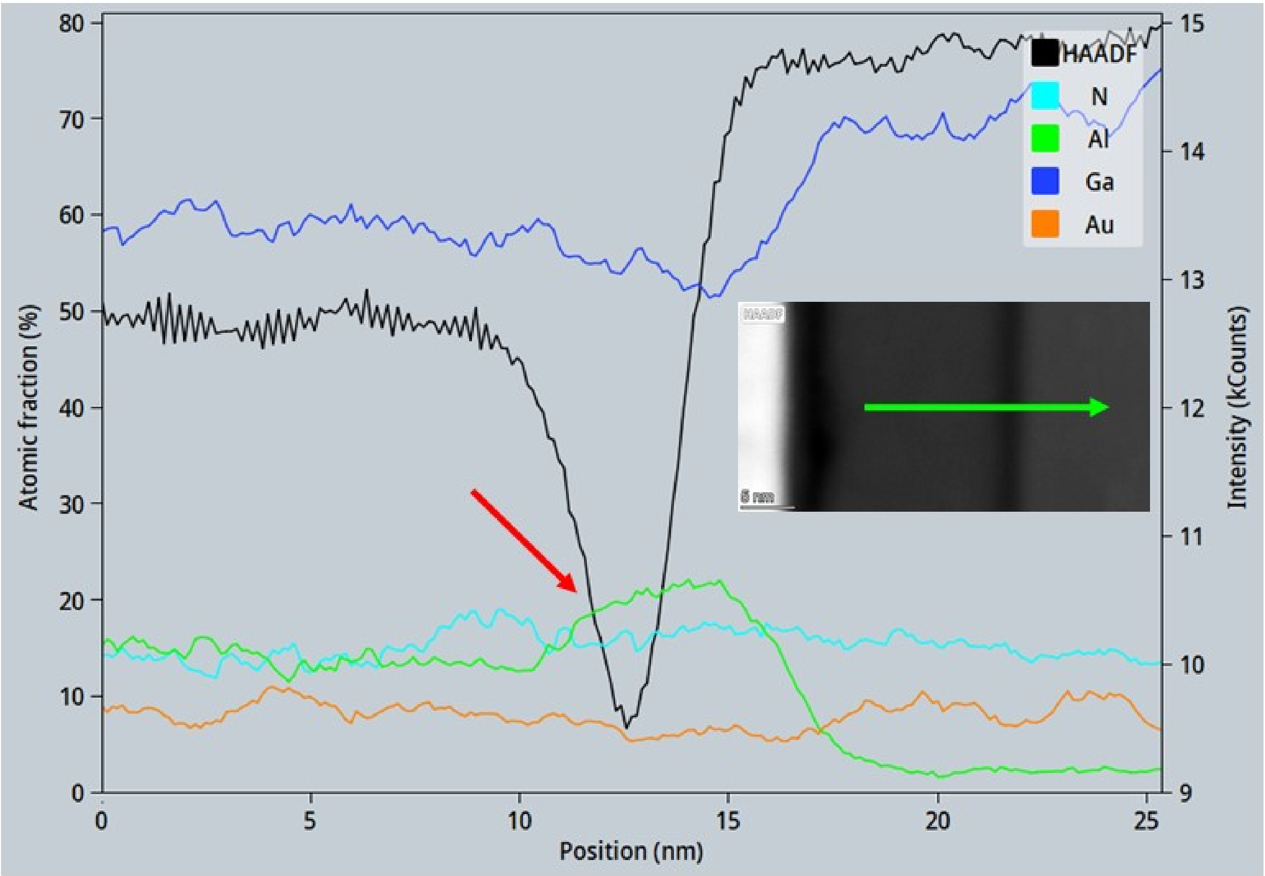

Figure S4 – HAADF and EDS intensity profiles (heterostructure **C**). The inset shows the corresponding STEM-HAADF image. The red arrows highlight the presence of the AlN interfacial layer. The green arrow highlights the direction used to determine the intensity profiles.

S2. HR-XRD structural analysis

Dislocation densities in the GaN and AlGaN epilayers, calculated using the commonly employed method that relies on the FWHM of ω scans,[S1] are listed in Table S1 – this has been done to compare with the method proposed by Kaganer.[S2] Dislocation densities are undervalued of (at least) one order of magnitude compared to the method proposed in reference [S2] – this being consistent with our previous work.[S3] Nevertheless, similar conclusions can be drawn. While the quality of GaN buffer layers remains consistent across the three heterostructures on one hand, it becomes even more evident that the inclusion of an AlN interlayer acts as a barrier, hindering the propagation of dislocations in the AlGaN epilayer on the other. The density of mixed dislocations in the AlGaN layer is reduced by half in the specimen containing a (nominal) 3 nm AlN interlayer – from 0.29×10^{10} cm^{-2} to 0.14×10^{10} cm^{-2}.

Table S1 – Dislocation densities in the GaN buffer, and AlGaN layer, reported as $\times 10^{10}$ cm^{-2}, and estimated according to the FWHM method.[S1] Edge and screw dislocation densities for AlGaN were calculated considering RCs around the (12.3) and (00.4) reflections, respectively.

	GaN FWHM			AlGaN FWHM		
Heterostructure	ρ_{edge}	ρ_{screw}	ρ_{mixed}	ρ_{edge}	ρ_{screw}	ρ_{mixed}
C | 3.0 nm	0.20	0.003	0.20	0.06	0.07	0.14
B | 1.5 nm	0.15	0.001	0.15	0.18	0.05	0.21
A | 0 nm	0.26	0.003	0.26	0.26	0.03	0.29

S3. Spectroscopic analyses: photoluminescence and cathodoluminescence

Table S2 – Al content in the AlGaN layers as estimated by the PL emission peak by using Vurgaftman and Nepal models. The exciton binding energy (in parenthesis) with the expected value for this material, has been added to the photoluminescence emission energy.

		Al (%)	
Heterostructure	**PL Emission (eV)**	**Vurgaftman [S4]**	**Nepal [S5]**
C | 3.0 nm	3.86 (+0.04)	18	22
B | 1.5 nm	4.10 (+0.04)	28	31
A | 0 nm	4.00 (+0.04)	24	29

CL findings for heterostructure **A** are presented in Figure S5. The presence of dark spots in CL maps of *c*-plane III-nitrides is widely regarded as indicative of the non-radiative activity associated with threading dislocations (see Figure S5a, orange full circle), as established in prior studies.[S6,S7] The CL signal observed near the dark spots (Figure S5a, dark-blue full circle) may result from near band gap emission,[S8] as shown by the dark-blue spectrum in Figure S5b, peaking at around 3.4 eV. However, the penetration depth profile obtained by simulations using the CASINO software suite,[S9] with the same parameters used to collect the CL intensity maps (1 nA and 5 keV), reveals that the signal mainly arises from the GaN buffer layer (see Figure S6). In this context, distinguishing the *shielding* effect of the AlN interlayer on the dislocation density within the AlGaN layer in the set of studied specimens is not feasible.

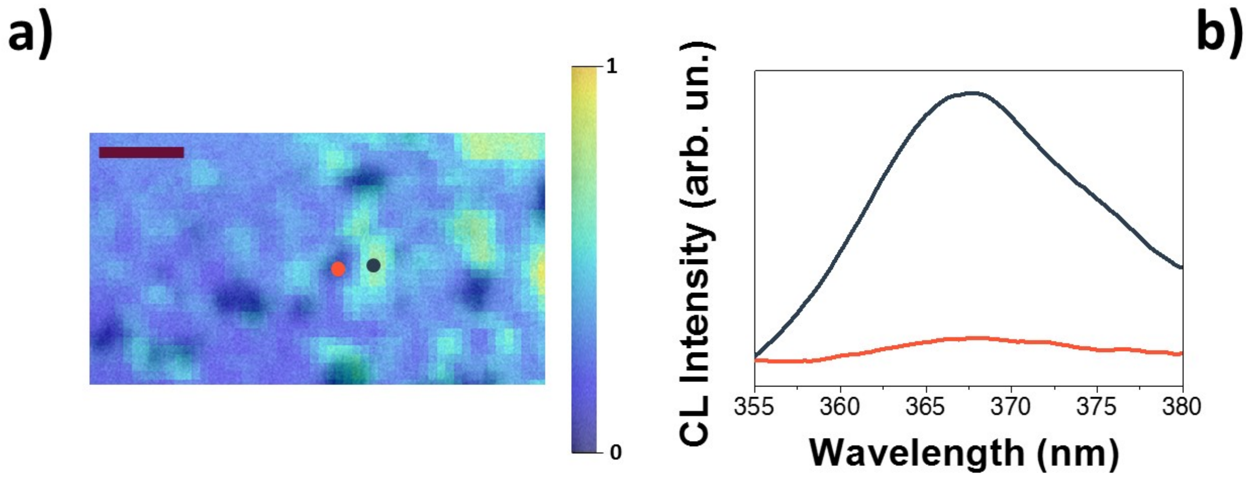

Figure S5 – a) CL integrated intensity map for heterostructure heterostructure **A**. The scale bar corresponds to 500 nm. b) CL spectra corresponding to the orange and dark-blue full circles in a).

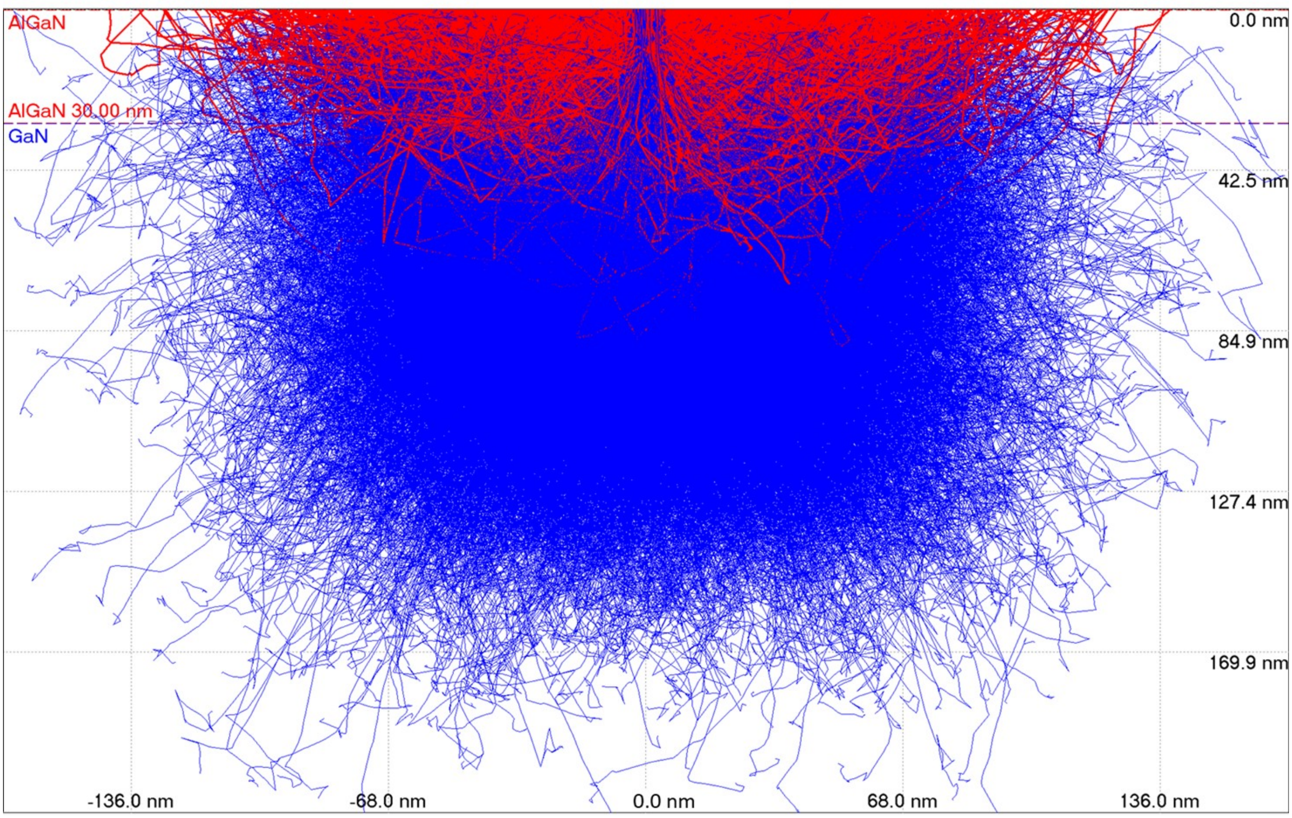

Figure S6 − Penetration depth profile in the *z*-direction computed by the CASINO software suite for the AlGaN/(AlN)/GaN heterostructure without the AlN interlayer, using the same parameters employed for collecting the CL intensity maps (1 nA and 5 keV). The red trajectories represent backscattered electrons, while the blue trajectories represent all other electrons capable of penetrating the material.

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