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Inversion of the Internal Electric Field in GaN/AlN Heterostructures Studied by Off-Axis Electron Holography

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Background incl. aims
Wurtzite III-nitride semiconductor are renowned for their applications in light emitting devices, due to their wide bandgap and doping capabilities. One of the main challenges of these materials is managing their intense spontaneous and piezoelectric polarization fields. In order to enhance the efficiency of GaN-based emitters, it is important to design new architectures to engineer the electric field in these materials. In addition, validation of these new designs requires the development of characterization methods capable of mapping the electric fields with nanometer resolution.

In this work, we study the effect of n-type delta doping on the potential profile of AlN/GaN and AlGaN/GaN superlattice using off-axis electron holography for the quantification of the electrostatic potentials. In addition, the sample composition, and the concentration and localization of dopants are determined using correlative techniques: high-resolution electron dispersive X-Ray spectroscopy (EDX), secondary ion mass spectroscopy (SIMS) and Nextnano simulations.

Methods
The samples under study consist of 10-periods of AlN/GaN (20 nm/20 nm) (1st series: samples S1 and S2) or 12 periods of AlN0.3Ga0.7N/GaN (15nm/15nm) (2nd series: samples S3, S4 and S5) grown by plasma-assisted molecular beam epitaxy. In the first series, S1 is non-intentionally doped and S2 is heavily doped with Ge in the GaN layers, at a nominal concentration [Ge] = 2.0±0.2 × 1021 cm−3, which is close to the solubility limit. In the second series, S3 is non-intentionally doped and S4 and S5 have a delta doping of Ge ([Ge] = 1020 cm-3) and Si ([Si] = 1019 cm-3), respectively, localized in the AlGaN layers. The dopant concentrations are measured by SIMS.

The electrostatic potential of the samples are measured by off-axis electron holography performed in a double-corrected FEI Titan Ultimate TEM operating at 200 kV. The electron holograms were recorded on a Gatan OneView 4k camera. EDX-spectroscopy was performed in a probe-corrected FEI Titan Themis microscope operated at 200 kV and equipped with a Super X detector system. EDX spectra quantification was done using the Cliff-Lorimer method.

Results
Using electron holography in undoped AlN/GaN and AlGaN/GaN samples (S1, S3), we confirm the presence of internal electric fields in the GaN and AlN layers, with a sign that is consistent with Schrödinger-Poisson simulations performed with the Nextnano software. Then, comparing S1 and S2, we are able to demonstrate the effect of carrier screening due to Ge doping. However, we also observed an inversion of the internal electric field in some of the AlN layers in S2. A correlative study involving holography, EDX and theoretical calculations of the band diagram demonstrate that this inversion can be attributed to Ge accumulation at the heterointerfaces in the AlN layers [1]. These result pave the way to the use of delta doping as a design tool to modulate and even invert the electric field in polar heterostructures.
The second sample series (S3, S4 and S5) presents our attempt to reproduce intentionally the inversion of potential observed in S2 by designing AlGaN/GaN heterostructures using delta

doping with silicon and germanium. In this case, we observe a systematic inversion of the internal electric field using Si doping. However, this inversion was not observed for Ge delta-doping. Further analysis using SIMS showed a migration of Ge in the GaN layer that explain this absence of inversion. This migration is consistent with our observations of a higher solubility limit of Ge in AlGaN compared with GaN [2], and is coherent with the Ge clustering observed in S2.

Conclusion

We show here that electron holography is a very powerful tool that allow the measurement of electrostatic potential with a nanometer resolution. It is particularly useful to study III-nitride materials that present peculiar electrostatic properties. We apply it here to study first the efficiency of germanium doping to screen the polarization-induced internal electric field in AlN/GaN superlattices. In addition, our identification of electric field inversion domains associated with Ge inhomogeneities paves the way for the use of delta doping as a tool in the design of heterostructures, to modulate and even invert the electric field in polar heterostructures. We have also addressed the effect of delta-doping in AlGaN/GaN, showing that inversion of the electric field is also possible using Si delta-doping, with improved reproducibility. Our studies show that the incorporation of germanium in III-nitride heterostructures remains challenging, with issues such as dopant segregation and dopant migration, but silicon delta-doping is also a very promising tool for fine-tuning of the internal electric fields in these materials.

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Graphic:

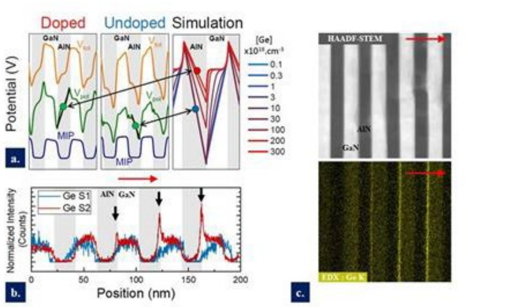

Fig.2: The red arrow represents the [0001] growth direction. [a] Comparison of the potential profiles for the doped (S2) and undoped (S1) potential with simulations (nextnano3 software), showing an inversion of the electric field in the AlN layer for the doped sample. [b] EDX profile of the germanium for S1 and S2. The signal observed for S1 is an artefact due to the proximity of Kα energy band for Ga and Ge. The black arrows highlight the Ge peak at AlN/GaN interfaces. [c] HAADF-STEM image of the AlN/GaN superlattice and EDX map of the Ge, showing the accumulation of Ge at interfaces.

Keywords:

Electron holography, III-nitride semiconductors, doping

Reference:

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[2] C. Bougerol, et al., ACS Appl. Mater. Interfaces 13, 4165 (2021)